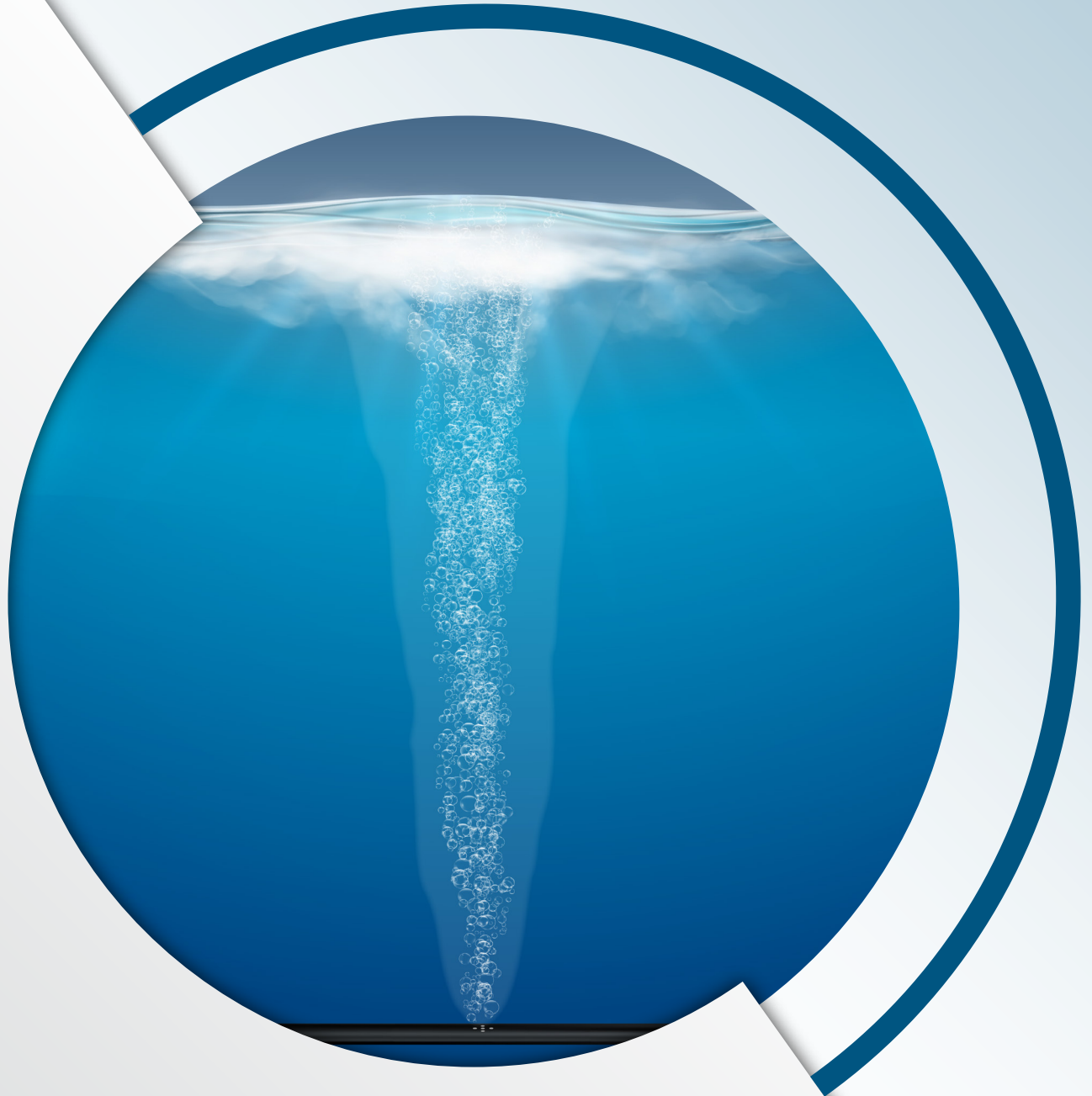




TUFLOW Water Quality User Manual

TUFLOW FV Water Quality (WQ) Module User Manual 2026.0

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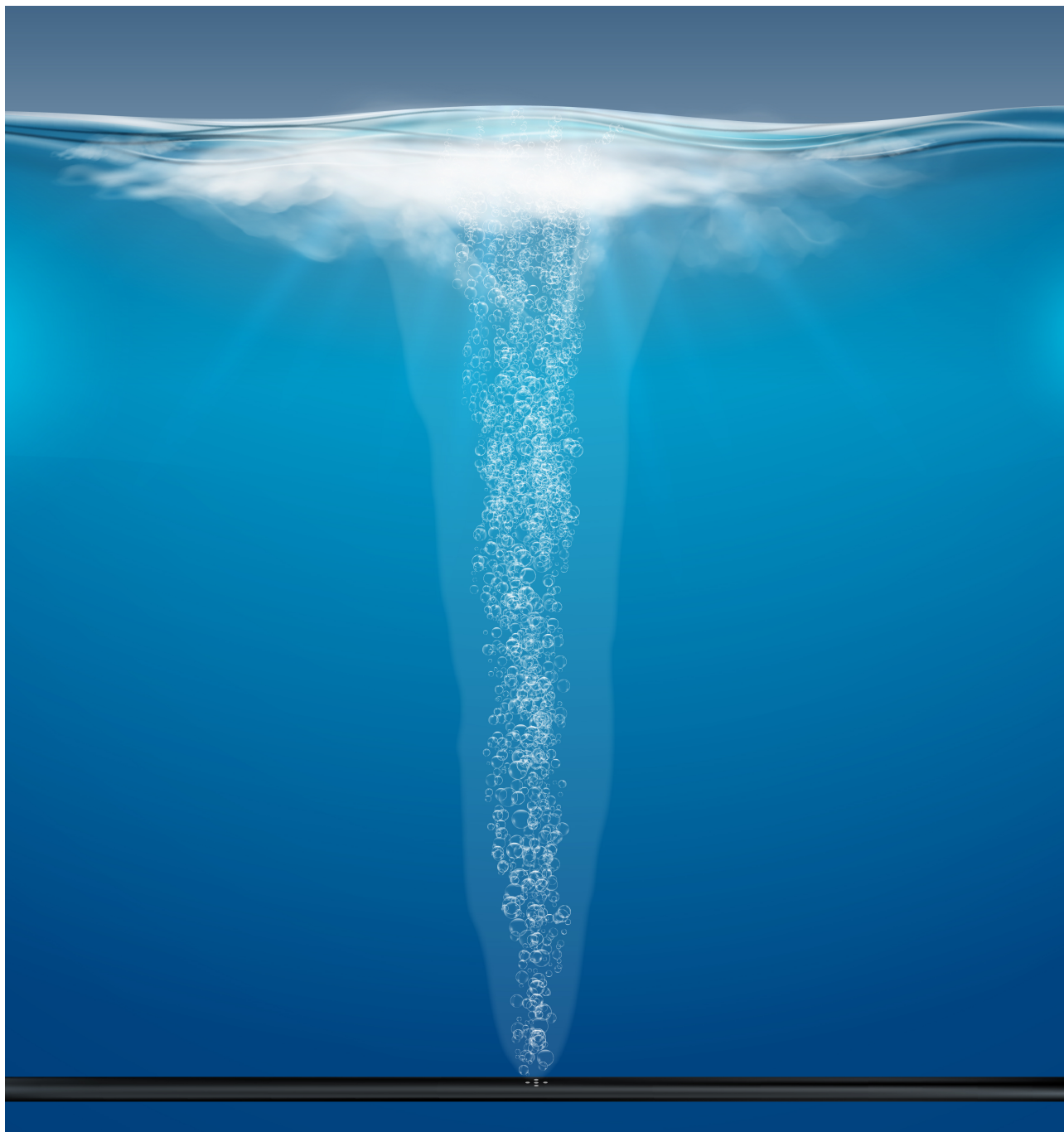
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TUFLOW FV Water Quality (WQ) Module User Manual



Overview

About this Manual

This document is the user manual for the TUFLOW Water Quality (WQ) Module.

Documentation for all previous releases, including archived manuals, is available from [TUFLOW Downloads](#).

How to use This Manual

This section provides an overview of the manual structure and the navigation features available to help locate information. These instructions are only provided in this section.

Structure

Model construction in the WQ Module follows a structured workflow. Users should begin with the [Architecture](#) chapter, which provides an overview of the WQ Module's core architecture. Following that, the [Process Descriptions](#) chapter provides a detailed description of the processes and capabilities of the WQ Module, together with a summary of its interactions with TUFLOW FV. Finally, the [Model Construction](#) chapter outlines the construction of a TUFLOW simulation with the WQ Module activated.

Several supporting appendices have been included in this manual. These contain interactive content to assist users in understanding and applying the WQ Module, beyond what might typically be included in a static user manual. These Appendices are interlinked and hyperlinked with content from the body of the manual where appropriate.

Navigation

This manual is organised into chapters, which are listed in the left sidebar. Select a chapter to navigate directly to that chapter. The top of the left sidebar also contains a search box which can be used to search the entire manual.

Within each chapter, the right sidebar displays a table of contents containing headings down to level 5 (e.g. Section 1.2.3.4.5). This provides an overview of the current chapter and allows navigation to a specific section. The current section is highlighted in bold as you scroll through the chapter.

At the bottom of each chapter, there are links to the previous and next chapters (when applicable).

The navigation bar at the top of the page provides quick access to the following features:

- Dark mode  : Toggle between light and dark themes
- PDF  : View the manual as a PDF document
- Reader mode  : Collapse or expand the left and right sidebars

Searching

The search function (top of the left sidebar) searches the entire manual, including chapters, tables, appendices and references. Matching results are displayed with a short preview of the surrounding text to help identify the relevant result before navigating to it.

Cross-references are used throughout the manual to link related content, including sections, figures, tables, equations, commands, etc. Hovering over a cross-reference displays a preview of the linked content. Selecting the link navigates directly to the referenced item.

Unit Systems

The WQ Module supports two unit systems: milligrams per litre (mg/L) and millimoles per cubic metre (mmol/m³). The unit system is specified via the `wq units` command. i.e. `wq units == mg/l` or `wq units == mmm`, respectively. The selected system determines how initial and boundary conditions are interpreted and which default parameter values apply.

In Appendix A, Appendix O and Appendix P, entries that support both unit systems display information for both of the systems in a small table. Only the row matching the simulation's unit system is applicable.

! Important

For a more detailed explanation of the two unit systems, see Section 4.2.

Commands

Commands are displayed in highlighted text and are often provided as a clickable link to their corresponding command description in Appendix A.

The command appendix provides detailed descriptions of each command and its parameters. Each command includes a summary block containing key information such as relevant construction section links. Command parameters are then described in individual sections (see [Parameters](#) for details). The table of contents in the right sidebar provides a convenient way to browse commands and parameters within the appendix.

TUFLOW commands use a structured, colour-coded syntax that is consistent throughout the documentation.

Colour coding:

- **Blue:** The command
- **Red:** The operator (`==`)
- **Black:** The input(s)/parameter(s)
- **Green:** Comments (must be preceded by `!`)

A vertical bar (`|`) separates the different input options for a command. For example, the following command has three options:

```
Simulation Class == DO | Inorganics | Organics ! command definition

Simulation Class == DO ! option 1 - Dissolved oxygen simulation class
Simulation Class == Inorganics ! option 2 - Inorganics simulation class
Simulation Class == Organics ! option 3 - Organics simulation class
```

For the Water Quality Module, most command inputs are parameters. As such, the usual default (`{ }`) and user defined (`<>`) syntax for inputs is not used and instead a more detailed description of the commands' parameter(s) is provided in subsections below the command.

For a detailed guide to reading a command entry in Appendix A, see the How to read a command entry section in that appendix.

Example command blocks are typically provided within scrollable code blocks. These blocks can be copied directly into a text editor when building a model control file. Select the  icon in the upper right corner of the block to copy the entire command block to the clipboard. An example block is provided below:

```
Simulation Class == DO ! Set simulation class to Dissolved Oxygen
WQ dt == 600.0 ! Set the WQ timestep (seconds)
WQ Units == Mg/L ! Set the units used for the WQ simulation
```

Parameters

Where commands specify computed variable parameters (e.g. half saturation concentrations, sediment fluxes etc.), they are referenced using their parameter notation (outlined below) rather than descriptive text. Parameter references are typically clickable links that navigate directly to the corresponding parameter description in Appendix A, where the parameter definition and description is provided.

In Appendix A, parameters are described following their corresponding command. Each parameter section has a description and a summary block with key information, such as default value, units, range and links to relevant science sections. Where a parameter supports two unit system options, information for both of the systems is displayed in a small table. Only the row matching the simulation's unit system is applicable. See [Unit Systems](#) for an explanation of the two unit systems.

! Important

Where parameter ranges are provided in Appendix A, these are not to be taken as fixed, but as indicative only. Some environmental settings may require parameterisation outside the ranges specified in this manual.

Parameter Notation

The primary groups of computed variable parameters are listed below, with the letter or symbol used to denote each. Typical generalisations of units are parenthesised.

- Fluxes, F (mass or moles per unit area or volume per unit time)
- Rates, R (per unit time)
- Concentrations, K (mass or moles per unit volume)
- Temperature coefficients, θ (dimensionless)
- Fractions, f (dimensionless decimal between 0.0 and 1.0)
- Ratios, X (dimensionless decimal that may be greater than 1.0, but always non-negative)
- Limitation functions, L (a dimensionless decimal between 0.0 and 1.0)
- Power exponents, P (typically dimensionless), and
- Velocities, V (metres per day)
- Boolean flags, B (either zero or one)

Typically (but not always) an instance of each of these groups will describe a computed variable and a process. Where appropriate, the computed variable and process are denoted as superscripts and subscripts, respectively. For example:

- The flux of oxygen across the sediment-water interface is notated as $F_{sed}^{O_2}$
- The rate of denitrification of nitrate is notated as $R_{denit}^{NO_3}$,
- The half saturation concentration of oxygen controlling the flux of filterable reactive phosphorus across the sediment-water interface is notated as $K_{sed-O_2}^{FRP}$
- The temperature coefficient controlling the flux of ammonium across the sediment-water interface is notated as $\theta_{sed}^{NH_4}$

In describing calculation processes (primarily in the Appendices) where a quantity is recomputed by the WQ Module as a direct modification of a user input or previously calculated quantity, then *(computed)* is used in the quantity's subscript. For example, a user can specify a sediment flux of ammonium, which is a parameter notated as $F_{sed}^{NH_4}$. The WQ Module can modify this parameter based on dynamic environmental conditions, and if so, the modified quantity is notated as $F_{sed(computed)}^{NH_4}$.

Computed Variables

Computed variables are the state variables tracked and advected by the WQ Module at every computational cell and timestep. Their concentrations are preserved between timesteps and are written to output files at the requested output times. Output computed variables are listed and described in Appendix O.

The unit systems described in [Unit Systems](#) applies to computed variables. For a guide to reading computed variable entries in Appendix O, see Section O.1.

Concentration values of computed variables refer to the elemental mass of the constituent rather than the molecular mass. See [Concentration Nomenclature](#) below for details.

Diagnostic Variables

Diagnostic variables are derived quantities computed during each WQ timestep, such as process rates and fluxes. Unlike computed variables, they are not tracked or advected between timesteps — each value is a snapshot of a rate or flux at a given instant. Diagnostic variables are listed and described in Appendix P.

The unit systems described in [Unit Systems](#) applies to diagnostic variables. For a guide to reading diagnostic variable entries in [Appendix P](#), see [Section P.1](#).

Concentration Nomenclature

Examples of processes and model simulations are provided in this manual, and these in turn refer to computed variable concentrations. These concentrations are denoted in square brackets, such as $[NO_3]$ for nitrate. The commonly accepted nomenclature for these variable concentrations is used in this manual, such as “nitrate concentration”. The numerical value of this concentration refers, however, to the concentration of elemental nitrogen within nitrate molecules: “6 mg/L of nitrate” means 6 mg/L of elemental nitrogen that is contained within nitrate molecules, not 6 mg/L of nitrate molecules. This is implicit in all references to all computed variables. More detail in this regard is provided in [Section 4.2](#), which should be reviewed carefully.

Interactive Figures

Some figures are interactive, allowing data to be explored directly within the manual. These figures support understanding of processes and the influence of specifiable parameters on water quality outcomes.

Note

In the PDF version of the manual, interactive figures are displayed as static images.

The figure below provides an example. Move the slider or press play to see the effect a sediment property has on water column concentrations. Zoom in by clicking and dragging out a box within the plot axes to be enlarged, and double click to return to the original axis limits. Mouse hover over a line on the figure to see plotted values.

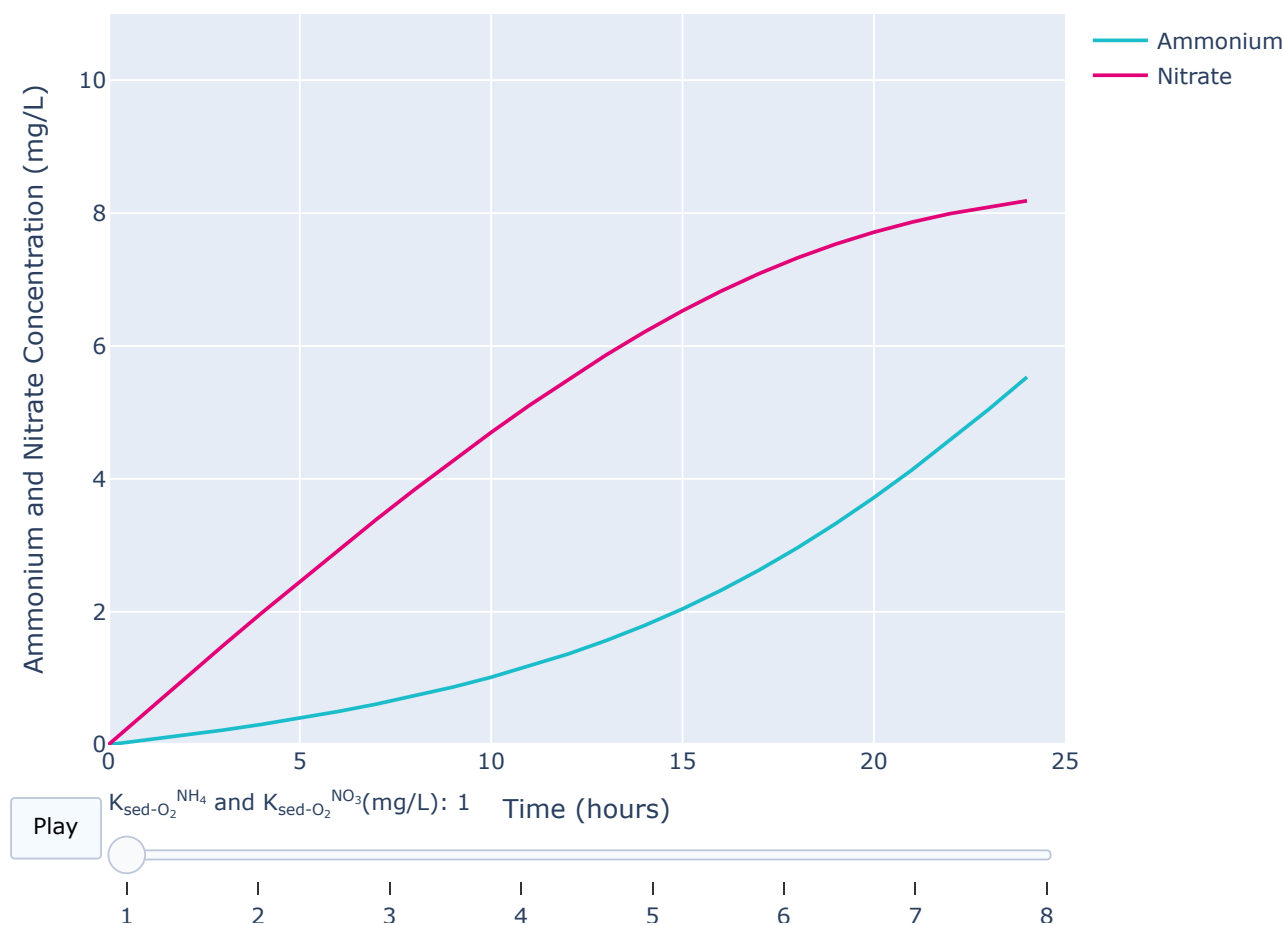


Figure 1

Interactive Networks

Interactive networks are used to illustrate simulation architecture and process descriptions. Networks comprise of nodes connected by lines, with interactive features.

Note

In the PDF version of the manual, interactive networks are displayed as static images.

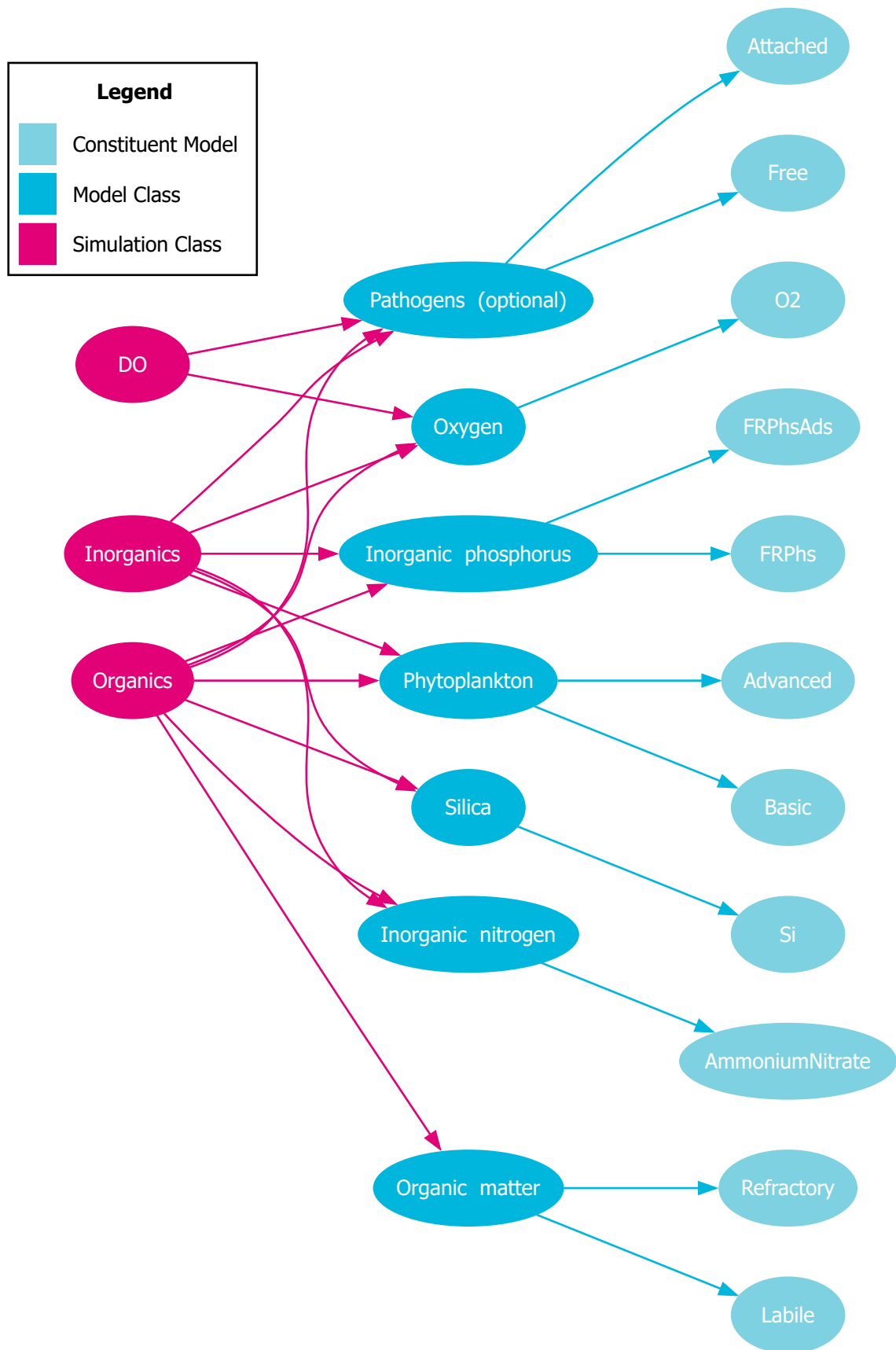
- **Architecture networks:**
 - Nodes represent items within water quality architectural levels.
 - Nodes are circular and coloured based on their architectural level:
 - * **simulation classes**
 - * **model classes**
 - * **constituent models**
 - * **computed variables**
 - Architectural relationships are displayed as connecting directional lines, with each line's colour matching that of its originating node
- **Process description networks:**
 - Nodes represent processes
 - Nodes are either:
 - * Circular processes nodes and are coloured as **sources** or **sinks** of computed variables. If a process is both source and sink, its **fill** and **outline** are coloured accordingly.
 - * Square computed variable nodes coloured as **computed variables**.
 - Process and computed variable relationships are displayed as connecting directional lines, with each line's colour indicating whether its direction is a **source** or **sink** with respect to its originating node.

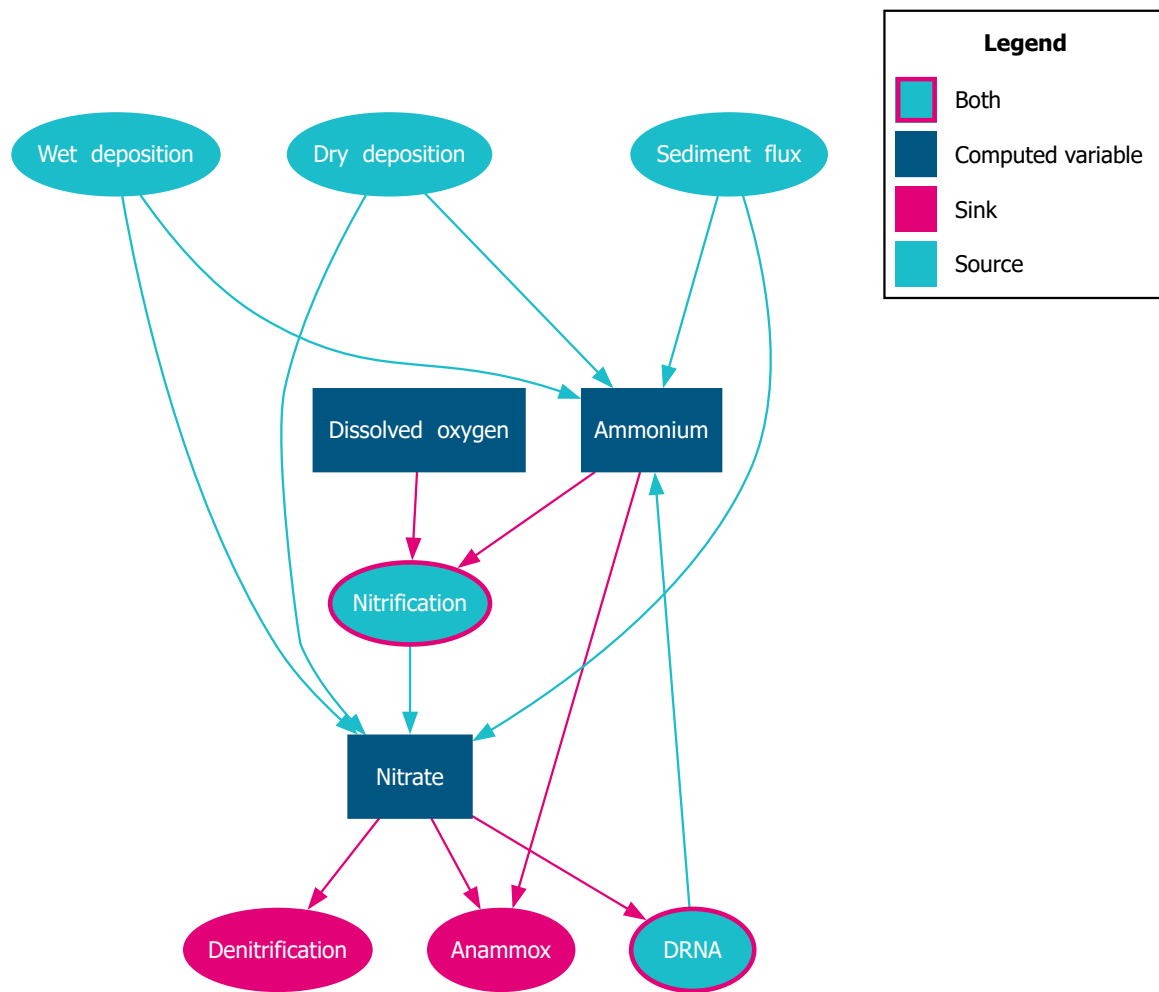
Connecting lines may have midpoint labels, and where present, these indicate indirect relationships to additional processes or computed variables.

Below are some tips for interacting with networks:

- Single click or hover over a node to highlight its nearest neighbours. Single clicking anywhere off the network will deselect these.
- Use the *Select by id* drop down menu to select a particular node of interest. Its nearest neighbours will also be automatically selected.
- Single click or hover over a legend entry to highlight all nodes of that type. Single clicking anywhere off the network will deselect these.
- Single click, hold and drag a node to move it.
- Single click, hold and drag white space anywhere within the activated network area to pan the entire network.
- Use the mouse wheel to zoom in and out of the network.
- Double click on any node that has the label starting text "Cluster on group :". This will explode the nodes to see its containing subsidiary nodes. To return to the original state, click the 'Re-initialise cluster' button on the bottom right of the frame.

Below are example architecture and process description networks to explore.





Feedback

Constructive suggestions to improve this manual are welcome, and can be emailed to support@tufLOW.com.

1 Introduction

1.1 Context

The TUFLOW FV Water Quality (WQ) Module enables the two- or three-dimensional simulation of water quality and ecological processes in natural and constructed waterways such as (but not limited to) lakes, tidal estuaries, river systems and coastal oceans. The module's design is flexible so as to support tailoring of its setup to meet individual application demands and complexity. The WQ Module is currently supported for use with **TUFLOW FV**, for releases from 2022 onward.

1.2 Features

1.2.1 Usability

Several key features have been included in the design of the WQ Module to support its use. Some are listed below.

- **Simulation units:** The units of simulation (including specification of initial conditions, boundary conditions and computed variable parameters) can be selected as either the commonly used mg/L (and $\mu\text{g/L}$ for phytoplankton) system, or the mmol/m³ system
- **Library defaults:** The WQ Module comes packaged with a fully populated library of default settings for all computed variable parameters. This means that users can quickly set up water quality simulations that automatically draw on these library defaults, with a view to then progressively overriding these defaults and therefore customising simulations to suit
- **Log file user feedback:** WQ Module simulations generate a log file that reports all simulation configuration details for review
- **Output computed variable names:** The WQ Module output variable names are descriptive and include the units used, for example WQ_DISS_OXYGEN_MGL
- **Output diagnostic variable names:** The WQ Module output diagnostic variable names are descriptive and include the units used, for example WQ_DIAG_O2_ATMOS_EXCHANGE_MG_M2_D
- **Specification of concentration limits:** The WQ Module allows users to optionally specify minimum and maximum concentration limits for each computed variable, and the WQ Module will reset concentrations to these limits if exceedences are detected. All instances of resetting are reported to the WQ Module log file as continuous commentary
- **Inbuilt guidance on parameter specification:** The WQ Module checks all user specified parameters and compares them to typical ranges. If a parameter's specified value falls outside a typical range, then a warning is reported to the WQ Module log file. These ranges are listed in Appendix A of this manual

1.2.2 Constituents and processes

Constituents currently simulated by the WQ Module include:

- Dissolved oxygen
- Silicate
- Inorganic nitrogen
 - Ammonium
 - Nitrate
- Inorganic phosphorus
 - Filterable reactive phosphorus
 - Adsorbed filterable reactive phosphorus
- Organic matter (labile and refractory)
 - Particulate organic carbon
 - Dissolved organic carbon
 - Particulate organic nitrogen

- Dissolved organic nitrogen
 - Particulate organic phosphorus
 - Dissolved organic phosphorus
 - Refractory dissolved organic carbon
 - Refractory dissolved organic nitrogen
 - Refractory dissolved organic phosphorus
 - Refractory particulate organic matter
- Phytoplankton (multiple groups)
 - Basic (excludes internal nutrient simulation)
 - Advanced (includes internal nutrient simulation)
- Pathogens (multiple groups)
 - Free (excludes attachment/detachment to sediment)
 - Attached (includes attachment/detachment to sediment)

Processes captured by the WQ Module include:

- Water column transformations between constituents (e.g. nitrification)
- Benthic sediment – water column interactions (e.g. sediment oxygen consumption)
- Atmospheric exchange (e.g. oxygen dissolution and rainfall deposition)
- Primary productivity, respiration and exudation of one or more phytoplankton groups
- Mortality, inactivation, settling and attachment/detachment of one or more pathogen groups

Future near-term releases of the WQ Module will include the ability to simulate:

- Macrophytes
- Particulate water quality constituents as sediment fractions (linked dynamically to TUFLOW FV's Sediment Transport (ST) Module)

Future mid-term releases will include:

- Zooplankton
- Biogeochemical particles (linked dynamically to TUFLOW FV's Particle Tracking (PT) Module)
- Sediment diagenesis
- Geochemistry

1.3 Science

The science underpinning the WQ Module is that developed at the School of Agriculture and Environment's **Oceans Institute** at **The University of Western Australia**. The WQ Module has wrapped this world class science into a form that is easily accessed via familiar TUFLOW style commands and workflows, and offers the additional features described in Section 1.2.1.

1.4 Support

BMT sells, distributes and supports the WQ Module. Contact support@tuflow.com or sales@tuflow.com for support and sales inquiries.



2 Architecture

This section provides a description of the WQ Module's architecture. This description is intentionally introductory, and details required to set up and execute simulations that deploy the WQ Module are provided in Chapter 4. The manual's introduction should be reviewed for instructions regarding the use of interactive components deployed in this manual.

2.1 Context

As our understanding of the natural environment advances, the questions asked of water quality and ecological numerical models are rapidly increasing in breadth and complexity. Setting up, calibrating and executing defensible environmental models has therefore become an increasingly challenging proposition.

The architecture of the WQ Module has been deliberately designed to assist users in overcoming some of these challenges, and in doing so improve the efficiency and effectiveness with which numerical modelling can support environmental management. Importantly, the WQ Module's architecture provides a mechanism by which users can rapidly initiate and execute water quality simulations without (at least in early modelling stages) concerning themselves with the often time consuming set up and parameterisation of simulated environmental processes.

In short, the WQ Module has been designed to provide immediate and easy access to its supporting state of the art environmental modelling science. The architecture that provides this easy access is tiered and these tiers are described below.

2.2 Simulation Tiers

The WQ Module's tiers are described below using the nomenclature of Figure 2.1. Every WQ Module simulation has the following tiers:

- **Tier 1:** Exactly one instance from a *simulation class*. This is user defined
- **Tier 2:** A suite of instances from a *model class*. The suite (and therefore number) of these instances is preset per simulation class. The exceptions to this are the phytoplankton and pathogen model classes, which when included in a simulation class can have as many instances within the suite as required by the user, with one instance (the default) per simulated phytoplankton or pathogen group
- **Tier 3:** Exactly one *constituent model* per model class instance (these are user selectable and there may be more than one constituent model available to choose from within a given model class instance)
- **Tier 4:** At least one *computed variable* per constituent model (the suite of computed variables is preset within each constituent model)

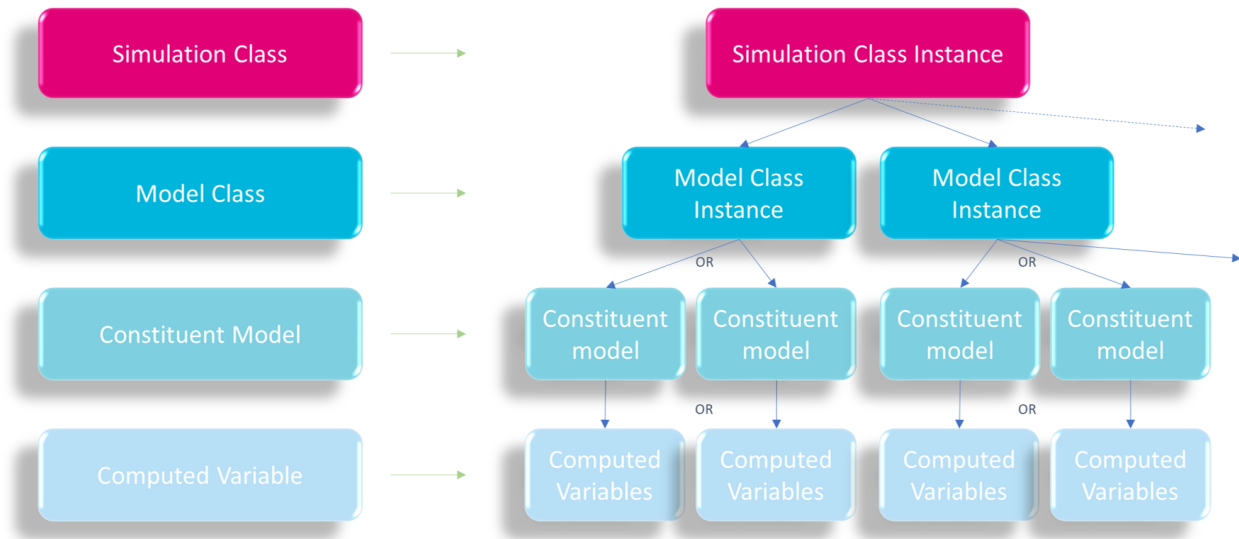


Figure 2.1: WQ Module tiers

Notwithstanding the above, a user need not specify any of the above in order to rapidly set up and execute a first pass WQ Module simulation. In this case, the WQ Module will automatically set the simplest instances of the simulation class, model classes, constituent models and computed variables by drawing on library defaults. Simulation tiers are described below.

2.2.1 Tier 1: Simulation Class

This is the highest and overarching tier of the WQ Module’s architecture. Using a single command, this tier sets the overall water quality simulation structure, including the suite of model classes to be deployed (with potentially multiple phytoplankton or pathogen model classes), and therefore the corresponding suite of constituent models and computed variables. The available simulation classes are provided in Table 2.1 as their keywords, together with example uses of each. The simulation class instances are cumulative, that is, a more complex class instance will include all the capability of simpler class instances. Complexity increases with table row in Table 2.1.

Table 2.1: WQ Module simulation class instances

Simulation Class Instance	Potential Uses
DO	Simulation of rudimentary dissolved oxygen dynamics such as: <ul style="list-style-type: none">• Desalination return water impact analyses• Seasonal reservoir oxygen analyses• Agricultural drain oxygen analyses
Inorganics	Simulation of relatively simple aquatic ecosystems that experience primary productivity such as: <ul style="list-style-type: none">• Shallow urban lakes• Smaller estuaries• Coastal ocean zones that are relatively free of organic materials or sediments• Mine voids
Organics	Simulation of more complex aquatic ecosystems such as: <ul style="list-style-type: none">• Impacted coastal embayments or nearshore zones• Impacted lakes• Larger estuaries• Wetlands• Aquaculture operations• Environments receiving point and/or diffuse source organic pollutants

Users can simply specify one preset simulation class (e.g. “organics”) in a water quality control file (Section 4.4 and following sections), and the WQ Module will draw on inbuilt library defaults to automatically construct and execute a water quality simulation, with no further user input required (beyond specification of water quality initial conditions, see Section 4.4.2). For example, a user may simply specify

```
Simulation Class == Organics
```

and initial conditions, and the WQ Module will construct itself, execute and report simulation details via a log file. This initial level of simplicity is intended.

2.2.2 Tier 2: Model Class

Each simulation class instance contains a preset suite of model class instances. These suites cannot be changed (although there may be multiple phytoplankton or pathogen model class instances), and are provided in Table 2.2 and as a network in Figure 2.2. For example, simulation class instance “Inorganics” has the fixed suite of oxygen, silicate, inorganic nitrogen, inorganic phosphorus and (potentially multiple) phytoplankton model class instances. The exception to this is pathogens. These can be optionally simulated in any simulation class (or none), and if simulated, potentially multiple pathogen model classes can be included.

Table 2.2: WQ Module simulation class instances and corresponding preset model class suites

Simulation Class Instance	Model Class Suite
DO	<ul style="list-style-type: none"> • Oxygen • Pathogens (optional, potentially multiple)
Inorganics	<ul style="list-style-type: none"> • Oxygen • Silicate • Inorganic Nitrogen • Inorganic Phosphorus • Phytoplankton (potentially multiple) • Pathogens (optional, potentially multiple)
Organics	<ul style="list-style-type: none"> • Oxygen • Silicate • Inorganic Nitrogen • Inorganic Phosphorus • Organic Matter • Phytoplankton (potentially multiple) • Pathogens (optional, potentially multiple)

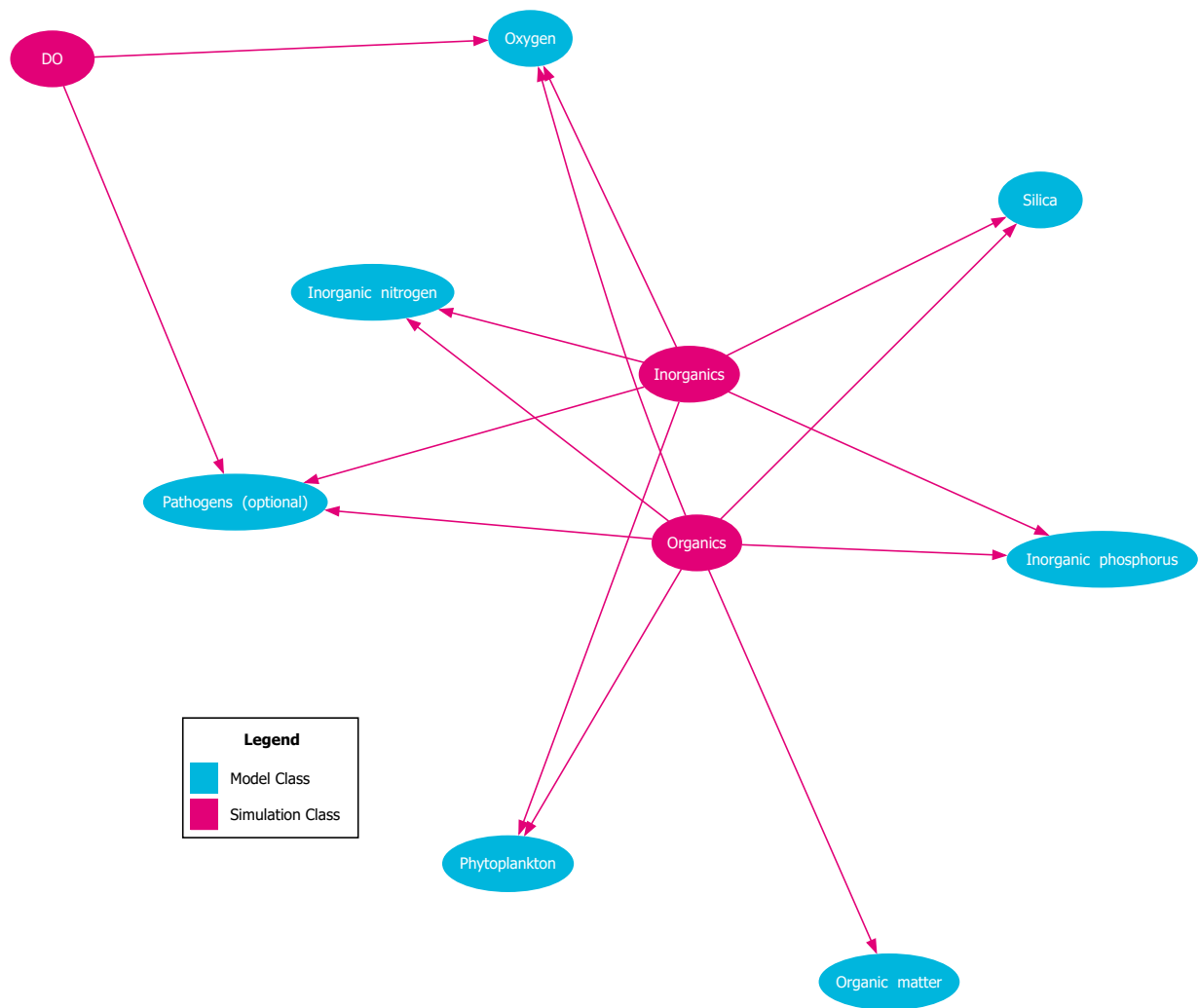


Figure 2.2: WQ Module simulation class and model class instances

2.2.3 Tier 3: Constituent Model

Whilst the suite of model class instances is set per simulation class instance, constituent models are interchangeable within a model class. In this way, a simulation class instance (at Tier 1) can be customised at the constituent model tier (at Tier 3), despite having a preset suite of model classes (at Tier 2, with potentially multiple phytoplankton and/or pathogen model class instances). Available constituent models are provided in Table 2.3, and presented graphically in Figure 2.3 as a direct extension of Figure 2.2. Pathogen model classes (and therefore constituent models) are always optional.

Table 2.3: WQ Module model classes and corresponding available constituent models

Model Class	Available Constituent Models
Oxygen	O2
Silicate	Si
Inorganic Nitrogen	AmmoniumNitrate
Inorganic Phosphorus	FRPhs FRPhsAds

Table 2.3: WQ Module model classes and corresponding available constituent models

Model Class	Available Constituent Models
Organic Matter	Labile
	Refractory
Phytoplankton	Basic
	Advanced
Pathogens	Free
	Attached

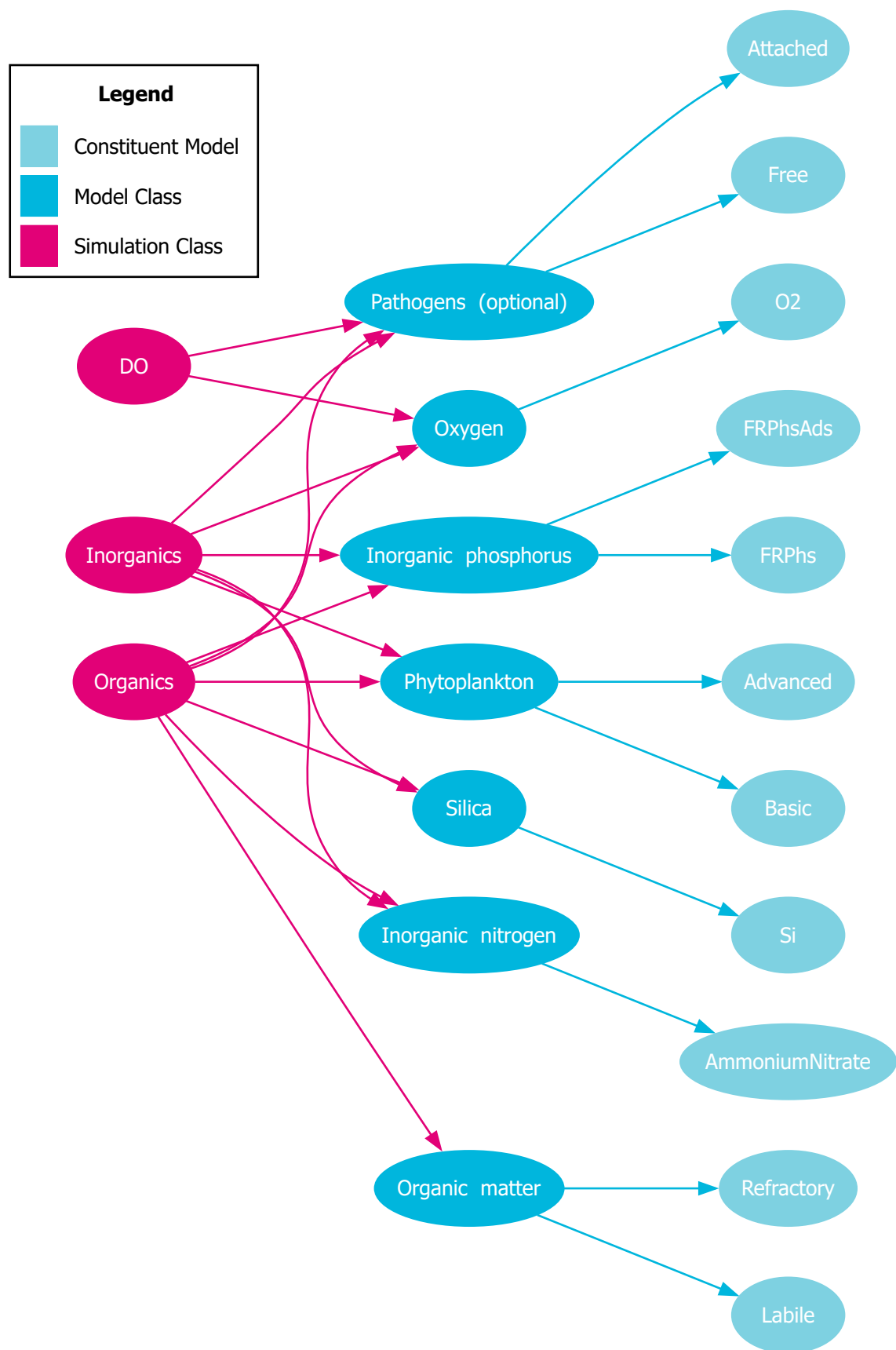


Figure 2.3: WQ Module simulation class and model class instances, with available constituent models

For example, multiple inorganic phosphorus constituent models are available within the inorganic phosphorus model class, where these models execute different water quality processes and contain different computed variables. In this example, this can be set with a single line command:

```
Inorganic Phosphorus Model == FRPhsAds
... commands ...
End Inorganic Phosphorus Model
```

This allows a user to interchange one phosphorus constituent model for another within the inorganic phosphorus model class, thereby customising the overarching simulation class instance.

The environmental processes simulated within each constituent model are fixed. Despite this, these processes can nonetheless be switched on and off as required, offering an additional layer of customisation. For example, if oxygen is not required to be included in silicate sediment flux calculations, the linkage between these processes and oxygen can be turned off by setting:

```
Oxygen == OFF
```

Alternatively, if a user wishes to simulate all inorganic processes other than nitrification for example, then the rate describing this unwanted process can simply be set to zero (as per the following command - the first numerical argument is the nitrification rate) and it will be turned off. All library defaults also set rate processes to zero.

```
Nitrification == 0.0, 0.0, 1.0
```

All processes included within each constituent model, and their respective WQ Module commands, are described in Chapter 3 and Chapter 4, respectively.

2.2.4 Tier 4: Computed Variables

Each Tier 3 constituent model contains a fixed set of computed variables. Table 2.4 (which is a direct extension of Table 2.3) provides the mapping between model classes, constituent models and their associated computed variables. These maps are also provided graphically in Figure 2.4, which is an extension of Figure 2.3, but presented in a non-hierarchical form. Click or hover over nodes to track their paths up or down the simulation tree.

For clarity, Figure 2.4 (and elsewhere within this manual) uses acronyms for some computed variable names, and these acronyms are expanded in Appendix O. All references in this manual to “organic matter” are to labile organic computed variables, unless specifically termed as refractory.

Table 2.4: WQ Module model classes, available constituent models and computed variables

Model Class	Available Constituent Models	Computed Variables
Oxygen	O2	Dissolved oxygen
Silicate	Si	Silicate
Inorganic Nitrogen	AmmoniumNitrate	Ammonium Nitrate
Inorganic Phosphorus	FRPhs FRPhsAds	Filterable Reactive Phosphorus (FRP) FRP Adsorbed FRP
Organic Matter	Labile Refractory	Labile dissolved and particulate organic carbon, nitrogen and phosphorus Labile dissolved and particulate organic carbon, nitrogen and phosphorus Refractory dissolved carbon, nitrogen and phosphorus and refractory particulate organic matter
Phytoplankton	Basic	Phytoplankton concentration and optionally cell density

Table 2.4: WQ Module model classes, available constituent models and computed variables

Model Class	Available Constituent Models	Computed Variables
Pathogens	Advanced	Phytoplankton concentration, internal nitrogen, internal phosphorus and optionally cell density
	Free	Pathogen alive and dead concentrations
	Attached	Pathogen alive, attached and dead concentrations

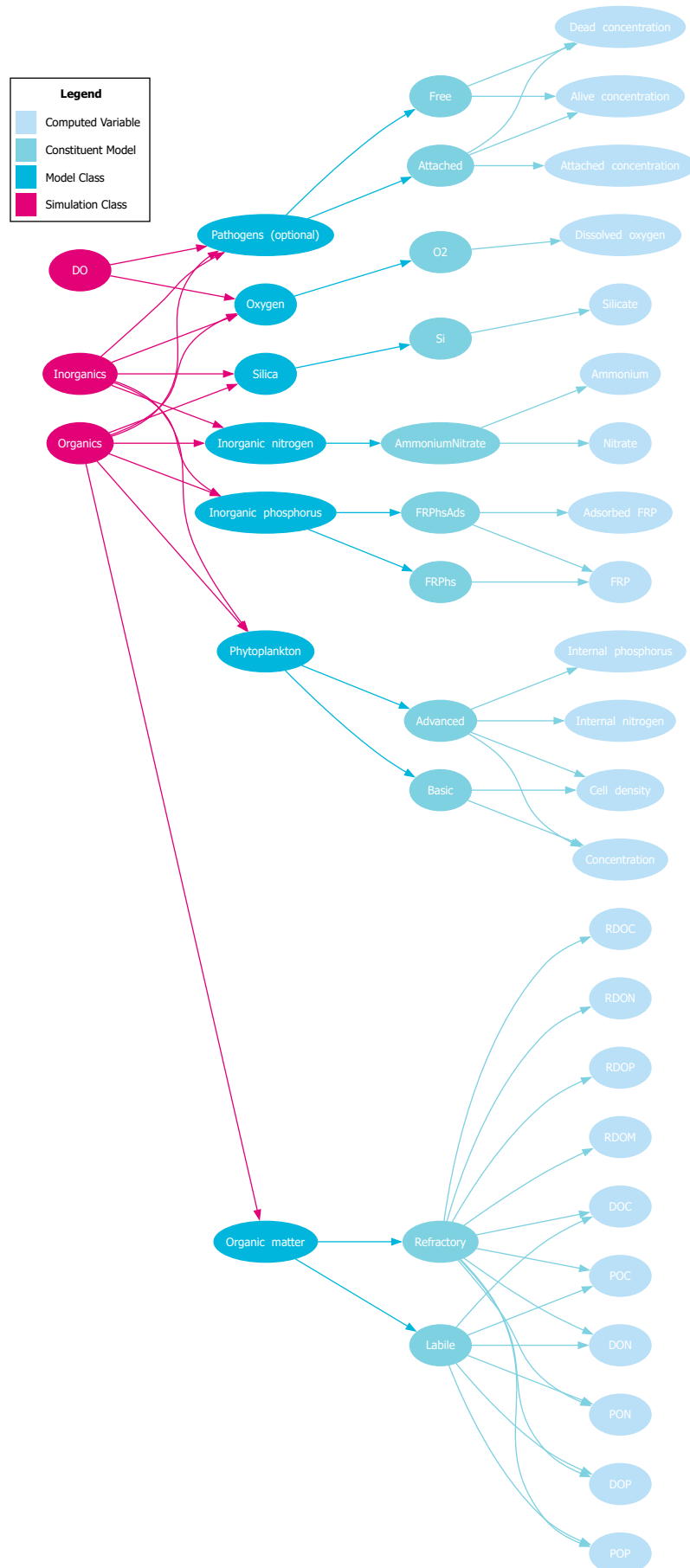


Figure 2.4: WQ Module simulation class and model class instances, available constituent models and computed variables

Parameters that govern the behaviour of computed variables are set within each constituent model. Parameters that are not set by the user are populated automatically from the WQ Module library defaults.

2.3 Linkage with TUFLOW FV

2.3.1 Process

Support is currently provided for linkage of the WQ Module with **TUFLOW FV**. Within this linkage, TUFLOW FV considers the WQ Module as a peripheral model with which it interacts at arm's length. The role of TUFLOW FV is that it (in approximate run time order):

- Requests the number of water quality constituents from the WQ Module at start up, based on user setup specifications (e.g. the setting of the simulation class instance, with any constituent model modifications)
- Automatically sets up the corresponding number of tracers (one for each computed variable) within its simulation (users do not specify these tracers)
- Is then responsible for the:
 - Application of WQ Module initial conditions
 - Conservative advection and dispersion of these tracers (that represent the WQ Module's computed variables)
 - Application of WQ Module boundary conditions
 - Calling the WQ Module at a user specified time step for the WQ Module to execute non-conservative transformation calculations on the suite of passive tracers
 - Writing of WQ Module results files

For example, if a WQ Module simulation was set to consider only dissolved oxygen, then TUFLOW FV would automatically allocate one tracer for the dissolved oxygen variable (the user does not need to specify passive tracers within TUFLOW FV), and advect and disperse that tracer throughout the model domain in response to initial and boundary conditions. At a user defined interval, TUFLOW FV would send the two- or three-dimensional tracer concentration field to the WQ Module for it to be modified in response to non-conservative ecological processes. The WQ Module would then return this modified tracer field to TUFLOW FV for subsequent advection and dispersion, with this exchange process continuing to simulation end.

2.3.2 Treatment of light

The TUFLOW FV heat module must be activated in order to use the WQ Module. One reason for this (beyond the need to compute water temperature) is that the heat module includes calculation of the light field within the model domain. This light field is used by various WQ Module constituent models.

In order to provide this light field, TUFLOW FV splits the shortwave radiation specified in the heat module into four bands:

- near infrared (NIR)
- photosynthetically available radiation (PAR)
- ultraviolet A (UVA), and
- ultraviolet B (UVB)

This split can be executed using TUFLOW FV defaults (recommended), or be user specified (not recommended). The corresponding band extinction coefficients in water with zero suspended sediment can also be specified in TUFLOW FV. Defaults are also available for all these coefficients and are recommended. TUFLOW FV uses these coefficients, along with other simulation properties, to compute the four light band intensities at the faces and centroids of each computational cell. The WQ Module uses the same split into bands as the TUFLOW FV defaults and ensures consistency in the treatment of light between TUFLOW FV and the WQ Module.

The WQ Module can also modify the light field sent to it from TUFLOW FV via calculation of phytoplankton self shading (Section [L.1](#)), the absorption of light due to the presence of organic matter and other processes. If this occurs, the WQ Module returns a modified light extinction coefficient field to TUFLOW FV that is then used in subsequent hydrodynamic heat and light calculations. This modification of light by water quality computed variables only occurs for simulation classes beyond DO.

2.4 Linkage with Other Hydrodynamic Models

The above communication between TUFLOW FV and the WQ Module is affected via implementation of a publicly available application programming interface (API). This API effectively sets the rules by which TUFLOW FV and the WQ Module communicate, and separates their roles.

This API has been designed so that TUFLOW FV can drive any other water quality model that includes the API in its compilation. This is intentional, and allows users of other ecological models to access the hydrodynamic power of TUFLOW FV for their simulations. Contact support@tuflow.com for further information or assistance in this regard.



3 Process Descriptions

Previous chapters have presented an overview of the architecture and capabilities of the WQ Module, together with a summary of its interactions with TUFLOW FV. This chapter presents the details of each simulation class (see Table 2.1) in terms of its available model classes, the constituent models within those model classes, and the associated computed variables.

Process descriptions are listed in this section primarily by name in tables and networks, without inclusion of detail. This is for clarity, with the detailed process descriptions and equations being provided in the Appendices. To facilitate this linkage with supporting material, each process tabulated in this section has been hyperlinked directly to the relevant Appendix, and these hyperlinks colour coded as [sources](#) or [sinks](#) relative to each computed variable presented.

Again for clarity, potential interactions of a computed variable with higher order computed variables (for example oxygen with phytoplankton) are included in this section only in descriptions of those higher order variables and processes. Further:

- Where a computed variable's process is modified by a lower order computed variable (e.g. silicate sediment flux modified by oxygen), then the lower order computed variable name is shown diagrammatically in a contrasting style overlying relevant process arrows in network diagrams
- Where a computed variable or process directly modifies a lower order computed variable (e.g. phytoplankton respiration consumes dissolved oxygen) then the lower order computed variable is explicitly included in tables and networks
- Computed variables listed in the tables are hyperlinked to supporting information in Appendix [O](#)
- Optional model classes (such as pathogens) are not included in the simulation class conceptual images (such as Figure 3.1) for clarity, but are first described in the simplest simulation class for which they can be deployed. Optional model classes are included in simulation class network diagrams only if they directly influence other water quality computed variables (e.g. pathogens do not, so are excluded from broader network diagrams).

The manual's introduction should be reviewed for guidance on the use of interactive components deployed in this section.

3.1 Simulation Class: DO

3.1.1 Overview

The intent of this simulation class is that it provide a relatively simple entry point to commence water quality modelling. There are many applications for this class. For example it might be used to examine basic oxygen dynamics across seasons in a water supply reservoir or a relatively newly constructed urban lake, or the potential impacts of dense desalination plant return waters on local coastal sediment oxygenation processes.

This simulation class includes only the oxygen model class as mandatory, but given oxygen's central role in environmental processes, it provides both a solid foundation for fundamental environmental investigations, and a platform from which to expand to more advanced simulation classes. The pathogens model class can be optionally included.

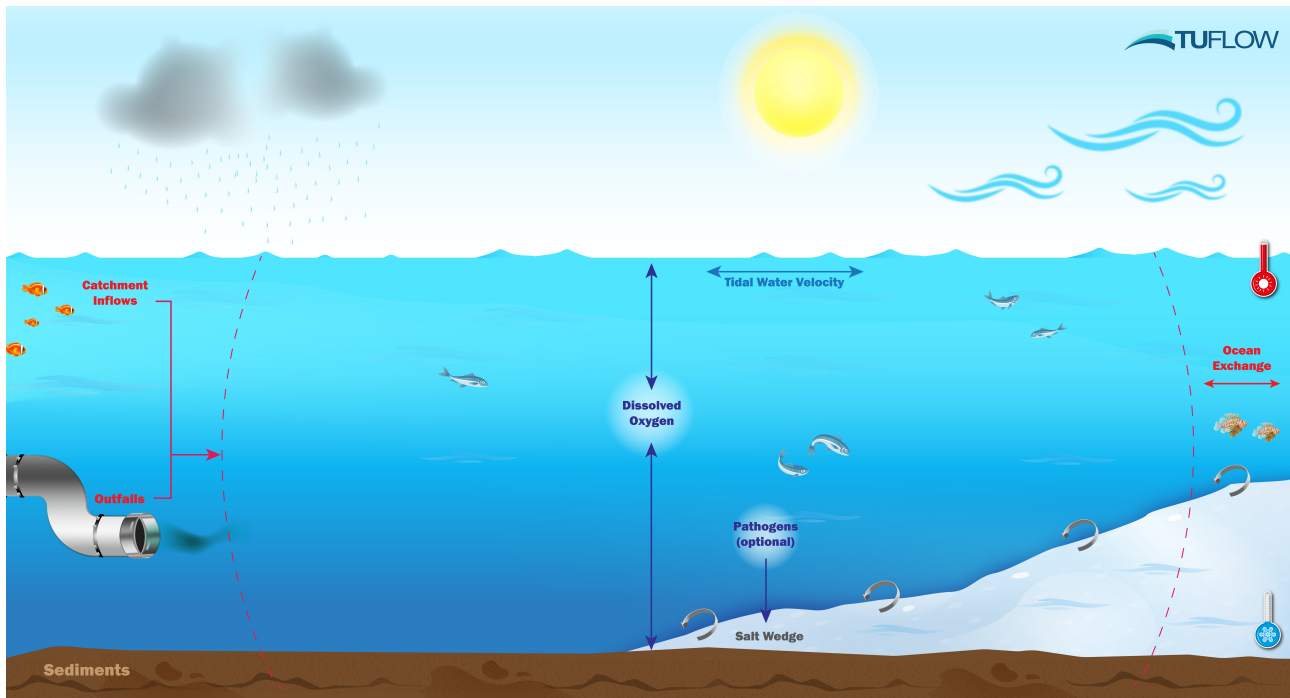


Figure 3.1: Simulation Class: DO (as an estuarine example)

3.1.2 Model Class: Oxygen

The following constituent models are available to select from within the oxygen model class.

3.1.2.1 Constituent Model: O2

The constituent model code and associated computed variables, processes and potentially interacting simulated quantities are provided in Figure 3.2 and Table 3.1.

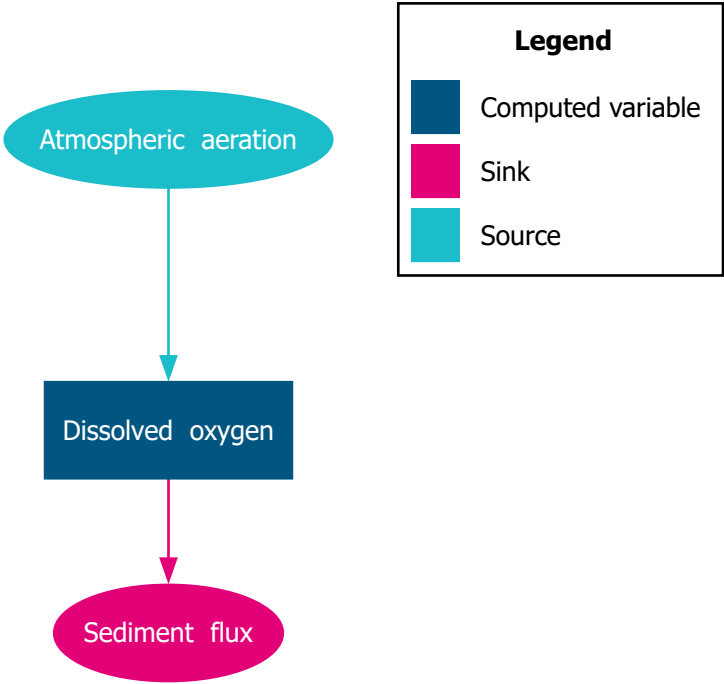


Figure 3.2: Constituent model: O2

Table 3.1: Constituent model properties - O2

Computed Variables	Units	Processes	Interacting Quantities
Dissolved Oxygen	mg/L or mmol/m ³	Atmospheric Aeration	• Wind speed
		Sediment Flux	• Dissolved oxygen
			• Water temperature
			• Dissolved oxygen
			• Sediment properties

In this relatively simple model, the only process requiring parameterisation is the sediment flux of oxygen.

3.1.3 Model Class: Pathogens (optional)

The following constituent models are available to select from within the pathogen model class.

3.1.3.1 Constituent Model: Free

The constituent model code and associated computed variables, processes and potentially interacting simulated quantities are provided in Figure 3.3 and Table 3.2.

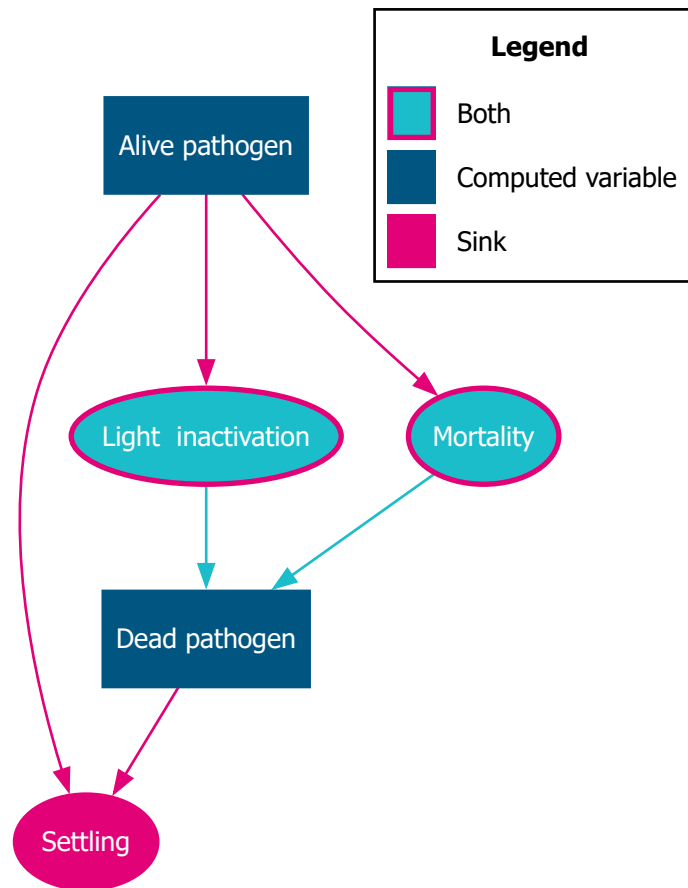


Figure 3.3: Constituent model: Free

Table 3.2: Constituent model properties - Free

Computed Variables	Units	Processes	Interacting Quantities
Alive Pathogen	CFU/100mL	Settling Mortality Light Inactivation Attachment Detachment	<ul style="list-style-type: none">Settling modelSalinityTemperatureMortality parametersLight and band splittingDOInactivation parametersAttachment parameters
Dead Pathogen	CFU/100mL	Settling Mortality	<ul style="list-style-type: none">Attachment parametersSettling modelSalinityTemperatureMortality parameters

Table 3.2: Constituent model properties - Free

Computed Variables	Units	Processes	Interacting Quantities
		Light Inactivation	<ul style="list-style-type: none">• Light and band splitting• DO• Inactivation parameters

3.1.3.2 Constituent Model: Attached

The constituent model code and associated computed variables, processes and potentially interacting simulated quantities are provided in Figure 3.4 and Table 3.3. This constituent model is the same as the Free constituent model, but allows for pathogens to attach to sediments.

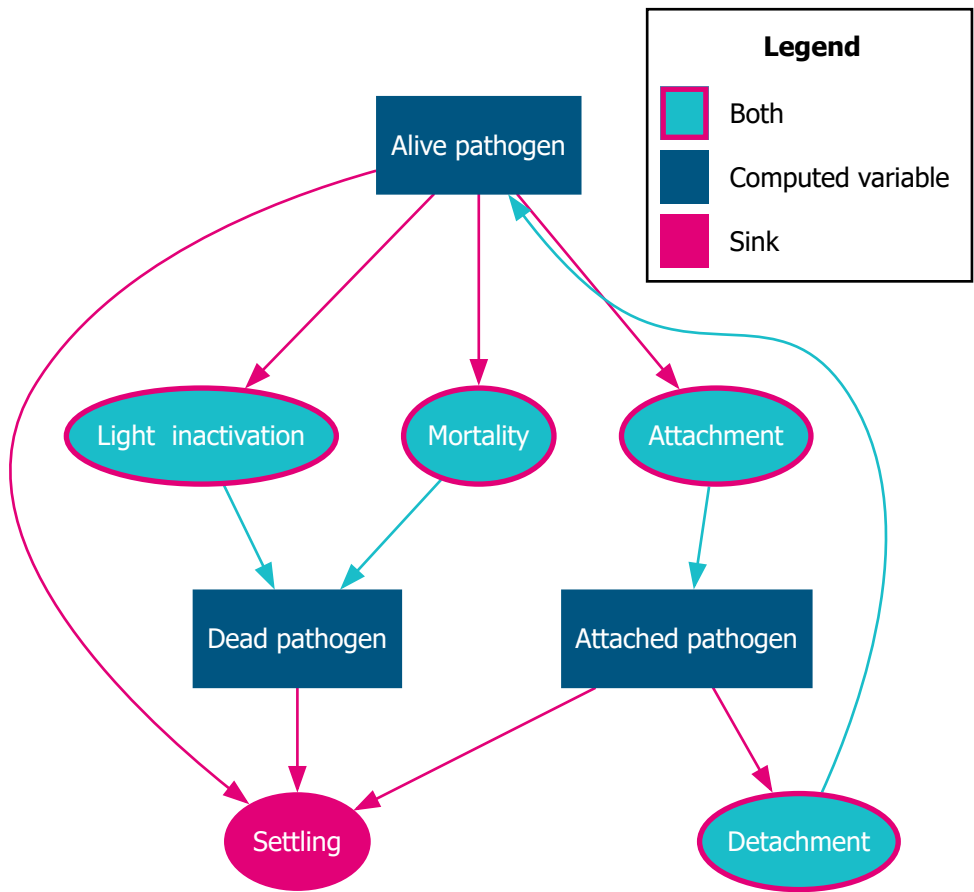


Figure 3.4: Constituent model: Attached

Table 3.3: Constituent model properties - Attached

Computed Variables	Units	Processes	Interacting Quantities
Alive Pathogen	CFU/100mL	Settling	<ul style="list-style-type: none">• Settling model

Table 3.3: Constituent model properties - Attached

Computed Variables	Units	Processes	Interacting Quantities
Dead Pathogen	CFU/100mL	Mortality	<ul style="list-style-type: none"> • Salinity • Temperature • Mortality parameters
		Light Inactivation	<ul style="list-style-type: none"> • Light and band splitting • DO • Inactivation parameters
		Attachment	<ul style="list-style-type: none"> • Attachment parameters
		Detachment	<ul style="list-style-type: none"> • Attachment parameters
		Settling	<ul style="list-style-type: none"> • Settling model
		Mortality	<ul style="list-style-type: none"> • Salinity • Temperature • Mortality parameters
		Light Inactivation	<ul style="list-style-type: none"> • Light and band splitting • DO • Inactivation parameters
		Attachment	<ul style="list-style-type: none"> • Attachment parameters
		Detachment	<ul style="list-style-type: none"> • Attachment parameters
Attached Pathogen	CFU/100mL	Attachment	<ul style="list-style-type: none"> • Attachment parameters
		Detachment	<ul style="list-style-type: none"> • Attachment parameters

Neither of the pathogen constituent models have complementary lower order computed variables, and their operation does not influence the concentrations of any other computed variables.

3.1.4 Computed variables

The only mandatory computed variable is this simulation class is dissolved oxygen, and as such the overarching simulation class network diagram is the same as that presented in Figure 3.2. If pathogens are simulated, then the corresponding simulation class network diagram is the (unconnected) aggregation of Figure 3.2 and either Figure 3.3 or Figure 3.4.

3.2 Simulation Class: Inorganics

3.2.1 Overview

The intent of this simulation class is that it provide a framework for simulating typical water quality conditions where organic matter does not play a significant role in ecosystem processes. For example it might be used to examine basic inorganic nutrient processing in nearshore coastal environments that include relatively unimpacted sandy bed conditions, or mine voids that receive little catchment inflow. This simulation class could equally be applied to smaller, well flushed estuaries that receive relatively little catchment derived organic matter, or to basic studies of lakes and water supply reservoirs. The latter cases (amongst others) might also use this simulation class as a stepping stone towards subsequent and more detailed simulations that include organic matter cycling. This would simply require upgrade from this simulation class to the organics simulation class.

This simulation class includes the oxygen, silicate, inorganic nitrogen, inorganic phosphorus, phytoplankton and (optionally) pathogen model classes.

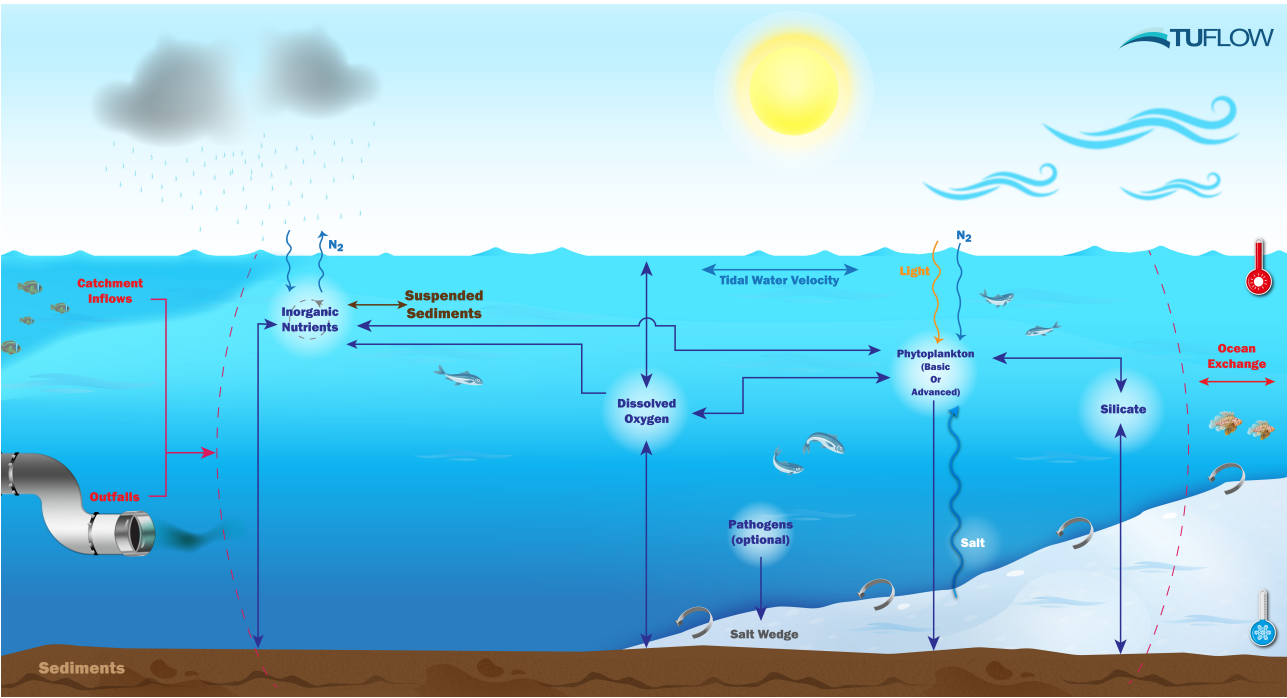


Figure 3.5: Simulation Class: Inorganics (as an estuarine example)

3.2.2 Model Class: Oxygen

This model class is the same as that described in Section 3.1.2.

3.2.3 Model Class: Silicate

The following constituent models are available to select from within the silicate model class.

3.2.3.1 Constituent Model: Si

The constituent model code and associated variables, processes and potentially interacting simulated quantities are provided in Figure 3.6 and Table 3.4.

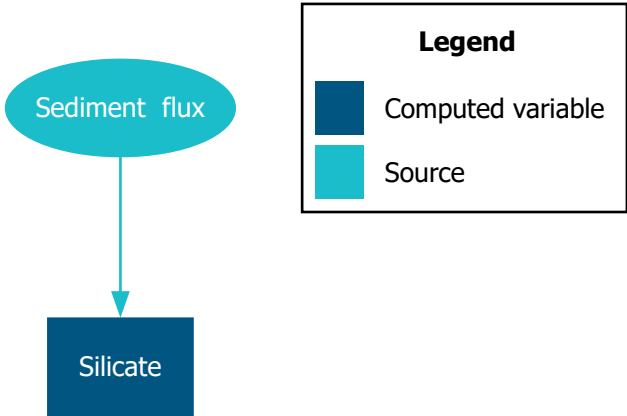


Figure 3.6: Constituent model: Si

Table 3.4: Constituent model properties - Si

Computed Variables	Units	Processes	Interacting Quantities
Silicate	mg/L or mmol/m ³	Sediment Flux	<ul style="list-style-type: none"> • Water temperature • Dissolved oxygen • Sediment properties

This is a relatively simple model, with the only process requiring parameterisation being the sediment flux of silicate. By default, this process depends on overlying dissolved oxygen concentrations, but this can optionally be turned off if required.

3.2.4 Model Class: Inorganic nitrogen

The following constituent models are available to select from within the inorganic nitrogen model class.

3.2.4.1 Constituent Model: AmmoniumNitrate

The constituent model code and associated variables, processes and potentially interacting simulated quantities are provided in Figure 3.7 and Table 3.5.

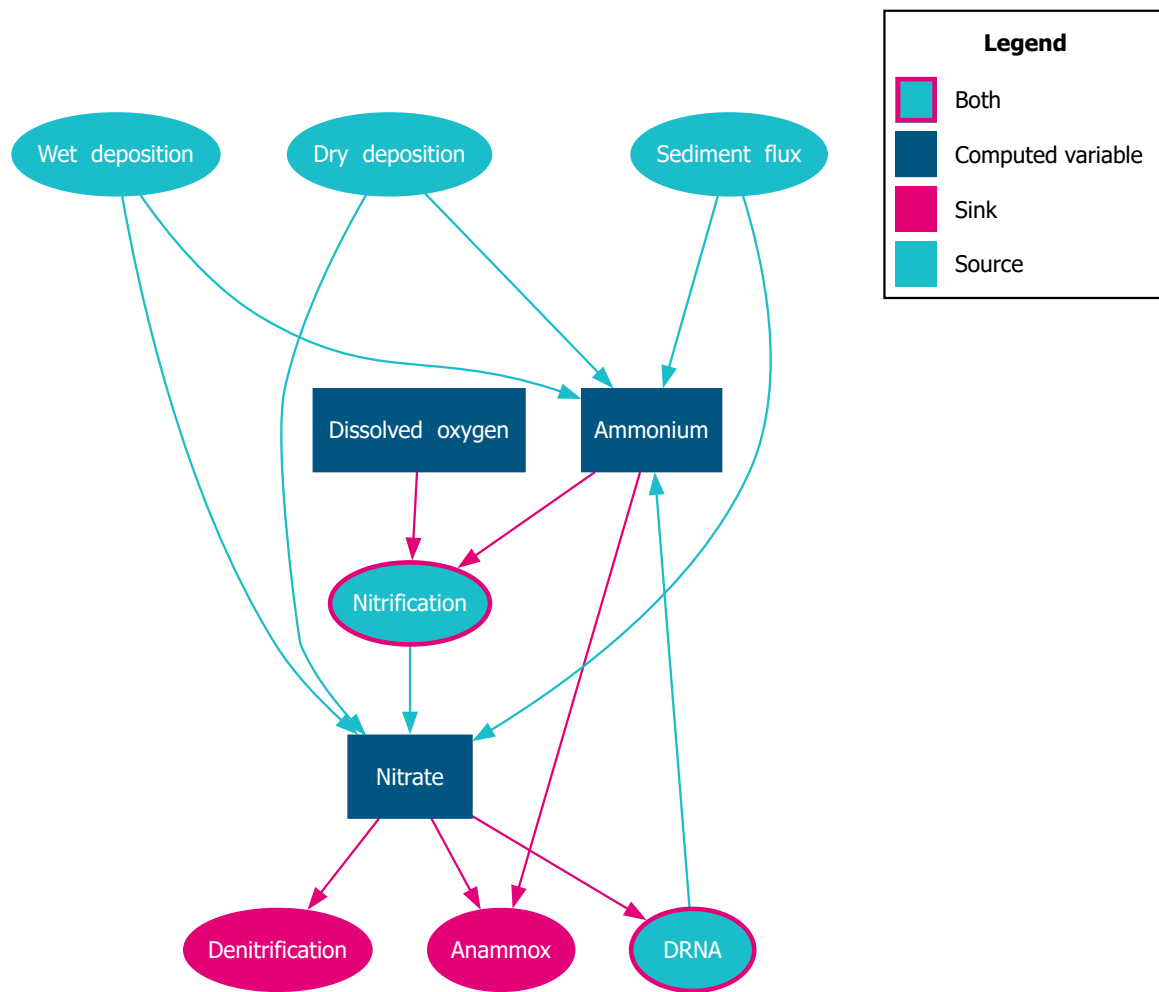


Figure 3.7: Constituent model: AmmoniumNitrate

Table 3.5: Constituent model properties - AmmoniumNitrate

Computed Variables	Units	Processes	Interacting Quantities
Ammonium	mg/L or mmol/m ³	Sediment Flux	<ul style="list-style-type: none"> Water temperature Dissolved oxygen Sediment properties
		Nitrification	<ul style="list-style-type: none"> Water temperature Dissolved oxygen Nitrification parameters Ammonium Rainfall
		Wet Atmospheric Deposition	
		Dry Atmospheric Deposition	<ul style="list-style-type: none"> Atmospheric parameters
		Anaerobic Oxidation of Ammonium	<ul style="list-style-type: none"> Dissolved oxygen Anammox parameters Ammonium Nitrate

Table 3.5: Constituent model properties - AmmoniumNitrate

Computed Variables	Units	Processes	Interacting Quantities
Nitrate	mg/L or mmol/m ³	Dissimilatory Reduction of Nitrate to Ammonium	<ul style="list-style-type: none"> Dissolved oxygen DNRA parameters
		Sediment Flux	<ul style="list-style-type: none"> Water temperature Dissolved oxygen Sediment properties
		Nitrification	<ul style="list-style-type: none"> Water temperature Dissolved oxygen Nitrification parameters Ammonium
		Denitrification	<ul style="list-style-type: none"> Water temperature Dissolved oxygen Denitrification parameters Nitrate
		Wet Atmospheric Deposition	<ul style="list-style-type: none"> Rainfall
		Dry Atmospheric Deposition	<ul style="list-style-type: none"> Atmospheric parameters
		Anaerobic Oxidation of Ammonium	<ul style="list-style-type: none"> Dissolved oxygen Anammox parameters Ammonium Nitrate
		Dissimilatory Reduction of Nitrate to Ammonium	<ul style="list-style-type: none"> Dissolved oxygen DNRA parameters

This is a slightly more complex model than those described previously, and this reflects the complexity of inorganic nitrogenous environmental chemistry. In addition to specification of two computed variables and their respective sediment flux properties, rates and related parameters for nitrification and denitrification are also specifiable. By design, the library defaults for these processes are set to zero so that all processes are initially inactive. Users may activate these processes by specifying non-zero rate parameters.

Whilst dissolved oxygen potentially modifies some processes described to this point (e.g. computed sediment flux rates), nitrification is the first of these processes that also potentially consumes dissolved oxygen. Specifically, if nitrification is simulated (i.e. non-zero rate parameters are specified) and allowed to include the effect of dissolved oxygen (the default), then dissolved oxygen concentrations are drawn down as the process operates.

Table 3.6: Complementary lower order computed variables - AmmoniumNitrate

Computed Variables	Units	Processes	Interacting Quantities
Dissolved Oxygen	mg/L or mmol/m ³	Nitrification	<ul style="list-style-type: none"> Water temperature Nitrification parameters Ammonium

3.2.5 Model Class: Inorganic phosphorus

The following constituent models are available to select from within the phosphorus model class.

3.2.5.1 Constituent Model: FRPhs

The constituent model code and associated variables, processes and potentially interacting simulated quantities are provided in Figure 3.8 and Table 3.7.

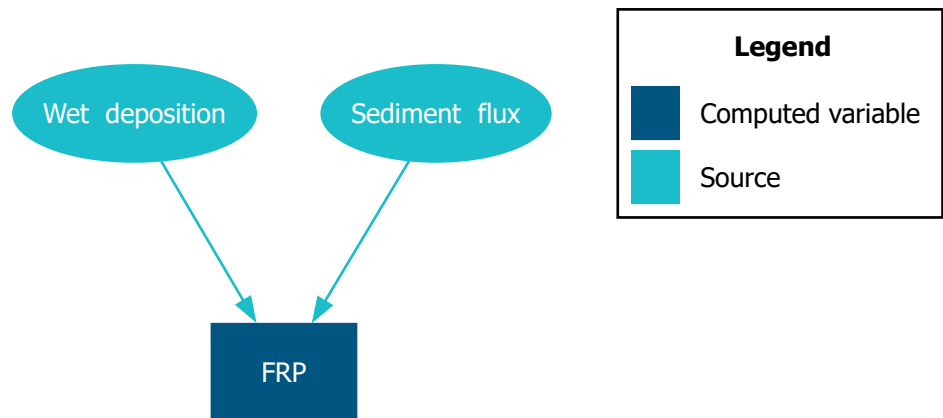


Figure 3.8: Constituent model: FRPhs

Table 3.7: Constituent model properties - FRPhs

Computed Variables	Units	Processes	Interacting Quantities
FRP	mg/L or mmol/m ³	Sediment Flux	<ul style="list-style-type: none">Water temperatureDissolved oxygenSediment properties
		Wet Atmospheric Deposition	<ul style="list-style-type: none">Rainfall

This is a relatively simple constituent model, but one that is critical to the simulation of higher order computed variables such as phytoplankton.

3.2.5.2 Constituent Model: FRPhsAds

The constituent model code and associated variables, processes and potentially interacting simulated quantities are provided in Figure 3.9 and Table 3.8.

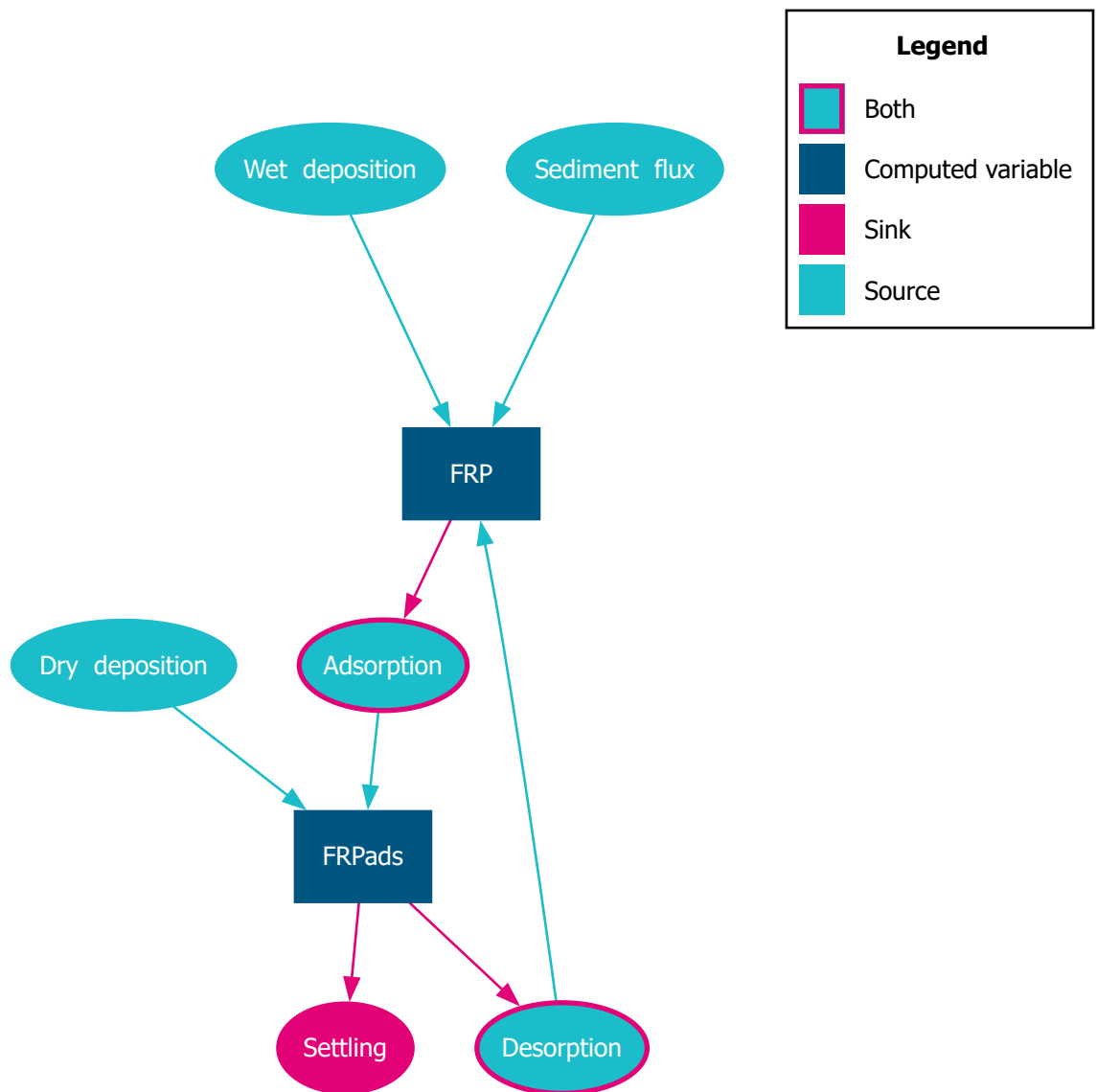


Figure 3.9: Constituent model: FRPhsAds

Table 3.8: Constituent model properties - FRPhsAds

Computed Variables	Units	Processes	Interacting Quantities
FRP	mg/L or mmol/m ³	Sediment Flux Wet Atmospheric Deposition Adsorption and Desorption	<ul style="list-style-type: none">Water temperatureDissolved oxygenSediment propertiesRainfallSuspended solidsFRPAdsorption parameters

Table 3.8: Constituent model properties - FRPhsAds

Computed Variables	Units	Processes	Interacting Quantities
FRP Adsorbed	mg/L or mmol/m ³	Adsorption and Desorption	<ul style="list-style-type: none"> Suspended solids FRP Adsorption parameters
		Settling	<ul style="list-style-type: none"> Suspended solids Suspended solids settling parameters
		Dry Atmospheric Deposition	<ul style="list-style-type: none"> Atmospheric parameters

In order for this constituent model to be used, the TUFLOW FV Sediment Transport (ST) Module must be activated to simulate at least one fraction of suspended sediment (several fractions may be so set). A WQ Module simulation will not start if the TUFLOW ST Module is not activated. In order to use this FRPhsAds constituent model therefore, the following must be in place:

- The TUFLOW FV ST Module must be activated and implemented
- At least one sediment fraction must be set up and executed within TUFLOW FV via the inclusion of a sediment control file, and specification of either of the following TUFLOW FV commands:

```
Include Sediment == 1,0 ! Do not include sediment in density calculations
```

or

```
Include Sediment == 1,1 ! Include sediment in density calculations
```

If multiple sediment fractions are specified to be simulated by the ST Module, then TUFLOW FV sends all these fraction concentrations as a sum through the API to the WQ Module, and this sum is used as the sediment concentration against which adsorption is computed. The WQ Module uses this information to compute FRP adsorption and loss of adsorbed FRP through settling. It is recognised that there are limitations of this approach. Future releases of TUFLOW FV and the WQ Module will address some of these limitations and allow for:

- User control of which ST Module sediment fractions are used in adsorption calculations, and
- Use of the TUFLOW FV ST Module settling and resuspension routines to dynamically link settling and resuspension of adsorbed FRP

3.2.6 Model Class: Phytoplankton

The following constituent models are available to select from within the phytoplankton model class. The differentiator between constituent models is the treatment of internal (to a phytoplankton cell) nutrient simulation.

3.2.6.1 Constituent Model: Basic

This basic phytoplankton constituent model assumes that the ratios of both internal nitrogen and phosphorus concentrations to internal chlorophyll *a* (or carbon) concentration are fixed. These internal nutrients are not simulated explicitly, but increase and decrease proportionately with increasing and decreasing carbonaceous biomass, according to the specified (or default) nitrogen-chlorophyll *a* and phosphorus-chlorophyll *a* (or their carbon equivalents) ratios. Carbonaceous biomass is simulated dynamically and is the measure of phytoplankton concentration. Internal nutrient concentrations are not required to be specified as initial or boundary conditions, and are not treated as computed variables.

The constituent model code and associated computed variables, processes and potentially interacting simulated quantities are provided in Figure 3.10 and Table 3.9. Silicate interactions only apply if phytoplankton is set to uptake silicate via specification of silicate limitation function parameters (Section 4.7.3.5.1). The configuration for phytoplankton simulation presented below applies only to the inorganics simulation class. A different, and expanded, configuration applies when phytoplankton is simulated using this basic constituent model in the organics simulation class. This expanded configuration is described in Section 3.3.7.1.

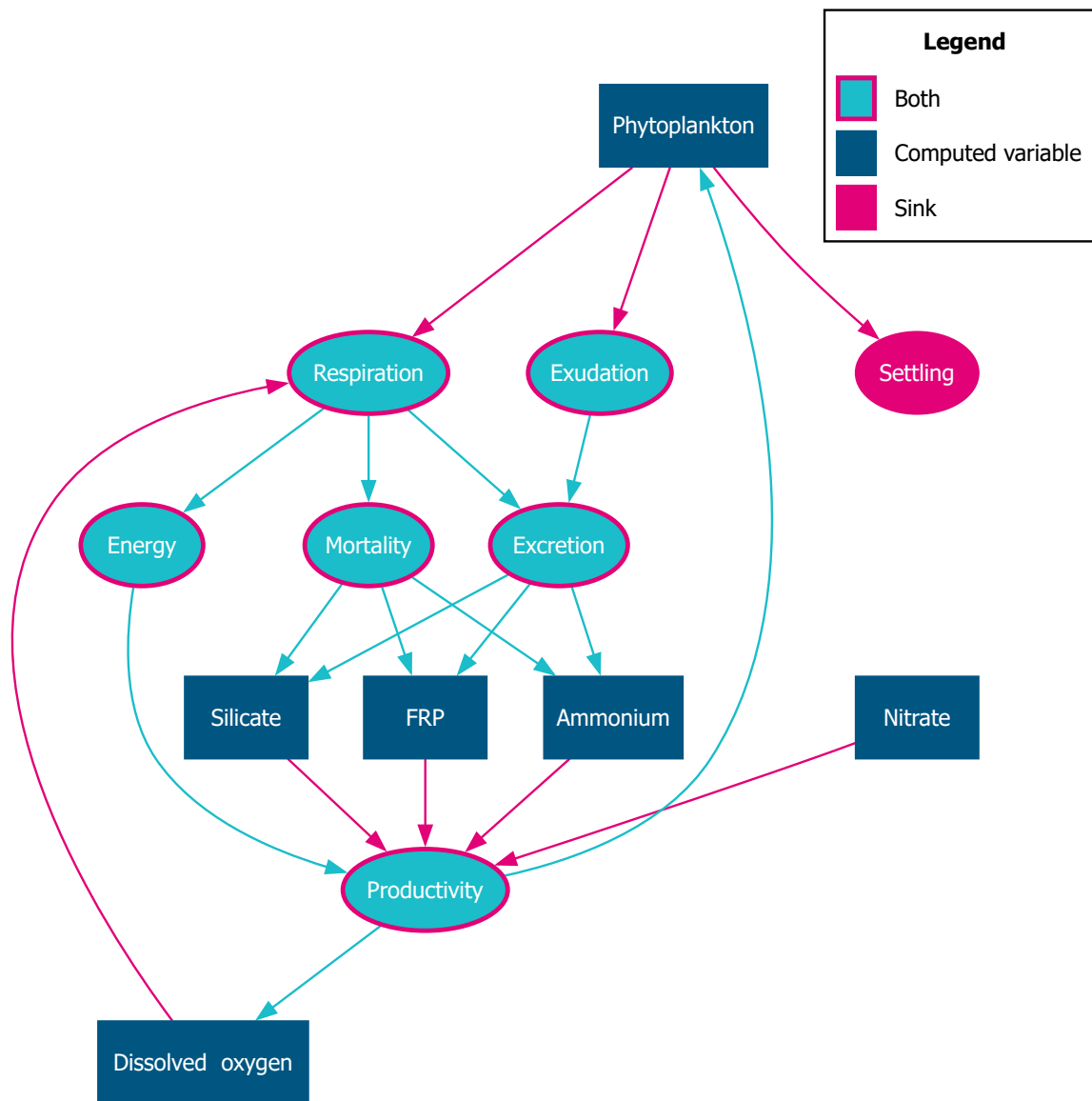


Figure 3.10: Constituent model: Basic

Table 3.9: Constituent model properties - Basic

Computed Variables	Units	Processes	Interacting Quantities
Phytoplankton	$\mu\text{g Chl } a/\text{L}$ or $\text{mmol C}/\text{m}^3$	Primary Productivity	<ul style="list-style-type: none">Water temperatureSalinityLightDissolved oxygenAmmoniumNitrateFRPSilicate (if activated)

Table 3.9: Constituent model properties - Basic

Computed Variables	Units	Processes	Interacting Quantities
		Respiration	<ul style="list-style-type: none"> Water temperature Salinity Light Dissolved oxygen
		Excretion	<ul style="list-style-type: none"> Ammonium FRP Silicate (if activated)
		Mortality	<ul style="list-style-type: none"> Ammonium FRP Silicate (if activated)
		Settling	<ul style="list-style-type: none"> Settling model Cell density

The three processes that govern phytoplankton behaviour are:

- Primary productivity (the photosynthetic conversion of light and carbon to stored energy and oxygen, also referred to as growth)
- Respiration (the expenditure of stored energy and oxygen), and
- Settling

A range of light, temperature, salinity, nitrogen, phosphorus and silicate limitation functions can be parameterised and applied in various combinations to the first two processes above, and a range of settling models are available to tailor the third. By design, the associated library default rates are set to zero so as to render all processes initially inactive. Specification of non-zero rates activates these processes.

The distinguishing property of this phytoplankton constituent model is that internal (phytoplankton cell) nutrient concentrations are considered to be fixed proportions of cell chlorophyll *a* (or carbon) concentrations. They are therefore not treated as computed variables, but rather as multiples of phytoplankton chlorophyll *a* (or carbon) (which is treated as a computed variable). The key implication of this is the method of calculation of the nitrogen and phosphorus uptake and limitation functions applied to primary productivity. These calculations depend only on ambient (i.e. external to a phytoplankton cell) water column nitrogen and phosphorus concentrations.

Simulation of phytoplankton dynamics in the inorganics simulation class directly modifies the concentrations of a range of other computed variables. These are listed in Table 3.10. Silicate interactions only apply if phytoplankton is set to uptake silicate.

Table 3.10: Complementary lower order computed variables - Basic

Computed Variables	Units	Processes	Interacting Quantities
Dissolved Oxygen	mg/L or mmol/m ³	Primary Productivity	<ul style="list-style-type: none"> Water temperature Salinity Light Ammonium Nitrate FRP Silicate (if activated)
		Respiration	<ul style="list-style-type: none"> Water temperature Salinity Light

Table 3.10: Complementary lower order computed variables - Basic

Computed Variables	Units	Processes	Interacting Quantities
Ammonium	mg/L or mmol/m ³	Primary Productivity	<ul style="list-style-type: none"> Water temperature Salinity Light Nitrate FRP Silicate (if activated)
		Excretion	<ul style="list-style-type: none"> FRP Silicate (if activated)
		Mortality	<ul style="list-style-type: none"> FRP Silicate (if activated)
Nitrate	mg/L or mmol/m ³	Primary Productivity	<ul style="list-style-type: none"> Water temperature Salinity Light Ammonium FRP Silicate (if activated)
FRP	mg/L or mmol/m ³	Primary Productivity	<ul style="list-style-type: none"> Water temperature Salinity Light Nitrate Ammonium Silicate (if activated)
		Excretion	<ul style="list-style-type: none"> Ammonium Silicate (if activated)
		Mortality	<ul style="list-style-type: none"> Ammonium Silicate (if activated)
Silicate (if activated)	mg/L or mmol/m ³	Primary Productivity	<ul style="list-style-type: none"> Water temperature Salinity Light Nitrate Ammonium FRP
		Excretion	<ul style="list-style-type: none"> Ammonium FRP
		Mortality	<ul style="list-style-type: none"> Ammonium FRP

3.2.6.2 Constituent Model: Advanced

This phytoplankton constituent model directly simulates internal (phytoplankton cell) nitrogen and phosphorus concentrations. These are allowed to vary between upper and lower limits, expressed as ratios to chlorophyll *a* (or carbon) concentrations. Internal nutrient concentrations (not as ratios) are required to be specified as initial and boundary conditions, and are treated as computed variables.

The constituent model code and associated variables, processes and potentially interacting simulated quantities are provided in Figure 3.11 and Table 3.11. Silicate interactions only apply if phytoplankton is set to uptake silicate. The configuration for phytoplankton simulation presented below applies only to the inorganics simulation class. A different, and expanded, configuration applies when phytoplankton is simulated using this advanced constituent model in the organics simulation class. This expanded configuration is described in Section 3.3.7.2.

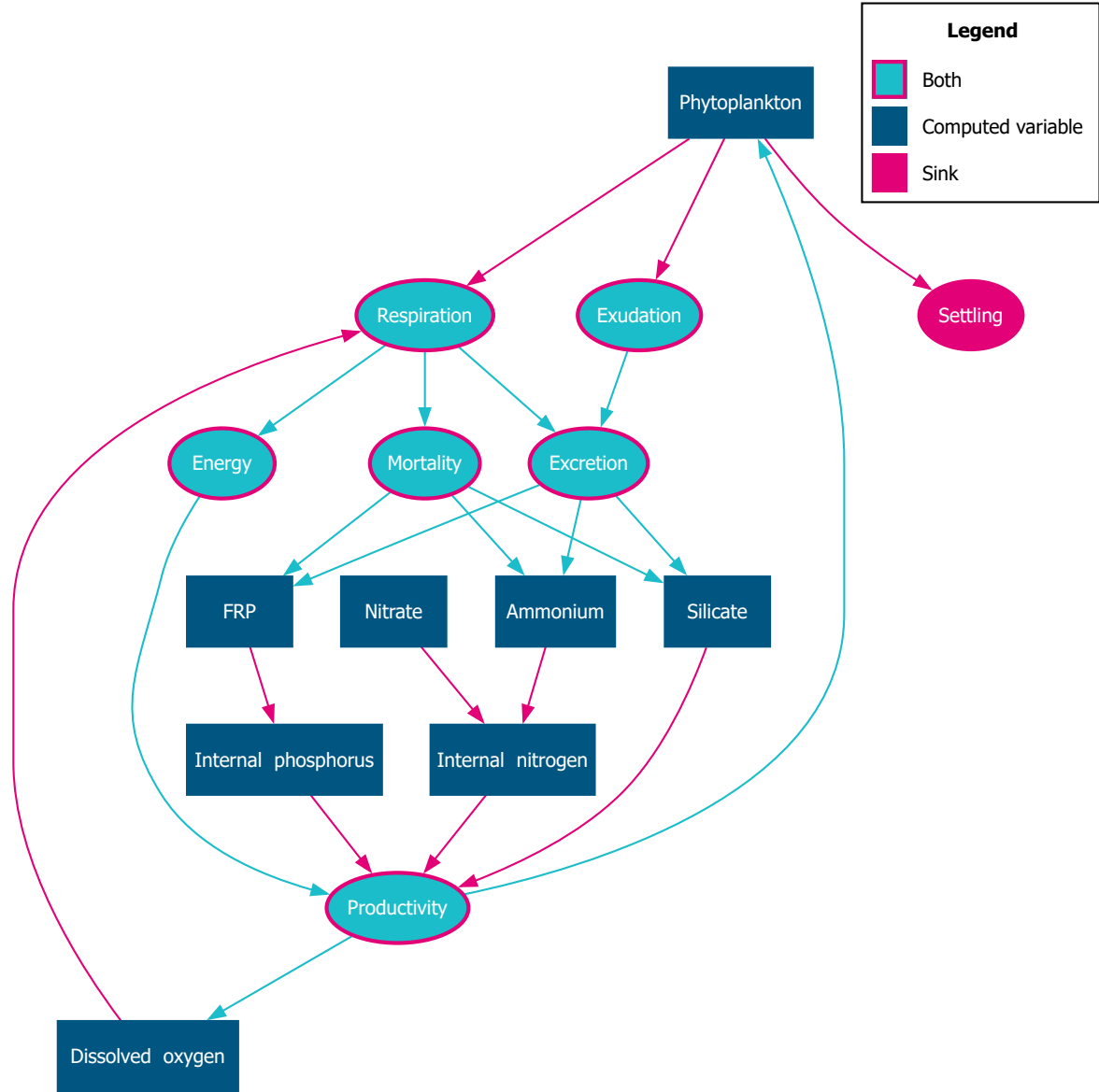


Figure 3.11: Constituent model: Advanced

Table 3.11: Constituent model properties - Advanced

Computed Variables	Units	Processes	Interacting Quantities
Phytoplankton	$\mu\text{g Chl } a/\text{L}$ or $\text{mmol C}/\text{m}^3$	Primary Productivity	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Dissolved oxygen • Ammonium • Nitrate • FRP • Internal nitrogen • Internal phosphorus • Silicate (if activated)
		Respiration	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Dissolved oxygen • Internal nitrogen • Internal phosphorus
		Excretion	<ul style="list-style-type: none"> • Ammonium • FRP • Internal nitrogen • Internal phosphorus • Silicate (if activated)
		Mortality	<ul style="list-style-type: none"> • Ammonium • FRP • Internal nitrogen • Internal phosphorus • Silicate (if activated)
		Settling	<ul style="list-style-type: none"> • Settling model • Cell density • Internal nitrogen • Internal phosphorus
Internal Nitrogen	$\text{mg N}/\text{L}$ or $\text{mmol N}/\text{m}^3$	Primary Productivity	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Dissolved oxygen • Ammonium • Nitrate • FRP • Internal phosphorus • Silicate (if activated)
		Uptake	<ul style="list-style-type: none"> • Water temperature • Ammonium • Nitrate • FRP • Internal phosphorus • Silicate (if activated)
		Respiration	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Dissolved oxygen • Internal phosphorus

Table 3.11: Constituent model properties - Advanced

Computed Variables	Units	Processes	Interacting Quantities
Internal Phosphorus	mg P/L or mmol P/m ³	Excretion	<ul style="list-style-type: none"> • Ammonium • FRP • Internal phosphorus • Silicate (if activated)
		Mortality	<ul style="list-style-type: none"> • Ammonium • FRP • Internal phosphorus • Silicate (if activated)
		Settling	<ul style="list-style-type: none"> • Settling model • Cell density • Internal phosphorus
		Primary Productivity	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Dissolved oxygen • Ammonium • Nitrate • FRP • Internal nitrogen • Silicate (if activated)
		Uptake	<ul style="list-style-type: none"> • Water temperature • Ammonium • Nitrate • FRP • Internal nitrogen • Silicate (if activated)
		Respiration	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Dissolved oxygen • Internal nitrogen
		Excretion	<ul style="list-style-type: none"> • Ammonium • FRP • Internal nitrogen • Silicate (if activated)
		Mortality	<ul style="list-style-type: none"> • Ammonium • FRP • Internal nitrogen • Silicate (if activated)
		Settling	<ul style="list-style-type: none"> • Settling model • Cell density • Internal nitrogen

The three processes that govern phytoplankton behaviour are:

- Primary productivity (the photosynthetic conversion of light and carbon to stored energy and oxygen, also referred to as growth)
- Respiration (the expenditure of stored energy and oxygen), and
- Settling

A range of light, temperature, salinity, nitrogen, phosphorus and silicate limitation functions can be parameterised and applied in various combinations to the first two processes above, and a range of settling models are available to tailor

the third. By design, the associated library default rates are set to zero so as to render all processes initially inactive. Specification of non-zero rates activates these processes.

The distinguishing property of this phytoplankton constituent model is that internal (phytoplankton cell) nutrient concentrations are simulated directly. They are therefore treated as computed variables. The key implication of this is the method of calculation of the nitrogen and phosphorus uptake and limitation functions applied to primary productivity. These calculations depend on both internal nutrient stores and ambient (i.e. external to a phytoplankton cell) water column nitrogen and phosphorus concentrations.

Simulation of phytoplankton dynamics in the inorganics simulation class directly modifies the concentrations of a range of other computed variables. These are listed in Table 3.12. Silicate interactions only apply if phytoplankton is set to uptake silicate.

Table 3.12: Complementary lower order computed variables - Advanced

Computed Variables	Units	Processes	Interacting Quantities
Dissolved Oxygen	mg/L or mmol/m ³	Primary Productivity	<ul style="list-style-type: none"> Water temperature Salinity Light Ammonium Nitrate FRP Internal nitrogen Internal phosphorus Silicate (if simulated)
		Respiration	<ul style="list-style-type: none"> Water temperature Salinity Light
Ammonium	mg/L or mmol/m ³	Primary Productivity	<ul style="list-style-type: none"> Water temperature Salinity Light Nitrate Internal nitrogen Internal phosphorus FRP Silicate (if simulated)
		Excretion	<ul style="list-style-type: none"> FRP Internal nitrogen Internal phosphorus Silicate (if simulated)
		Mortality	<ul style="list-style-type: none"> FRP Internal nitrogen Internal phosphorus Silicate (if simulated)
Nitrate	mg/L or mmol/m ³	Primary Productivity	<ul style="list-style-type: none"> Water temperature Salinity Light Ammonium Internal nitrogen Internal phosphorus FRP Silicate (if simulated)

Table 3.12: Complementary lower order computed variables - Advanced

Computed Variables	Units	Processes	Interacting Quantities
FRP	mg/L or mmol/m ³	Primary Productivity Excretion Mortality	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Nitrate • Ammonium • Internal phosphorus • Silicate (if simulated) • Ammonium • Internal nitrogen • Internal phosphorus • Silicate (if simulated) • Ammonium • Internal nitrogen • Internal phosphorus • Silicate (if simulated)
Silicate (if simulated)	mg/L or mmol/m ³	Primary Productivity Excretion Mortality	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Nitrate • Ammonium • FRP • Internal nitrogen • Internal phosphorus • Ammonium • FRP • Internal nitrogen • Internal phosphorus • Ammonium • FRP • Internal nitrogen • Internal phosphorus

3.2.7 Model Class: Pathogens (optional)

This model class is the same as that described in Section 3.1.3.

3.2.8 Computed variables

The relationships between all available computed variables and processes in this inorganics simulation class are presented in Figure 3.12. Depending on the constituent model classes deployed, not all of the computed variables and processes shown in the figure will necessarily be active. All network link labels have been removed (other than denoting the relevant phytoplankton model), and optional non-interacting model classes (e.g. pathogens) omitted, for clarity.

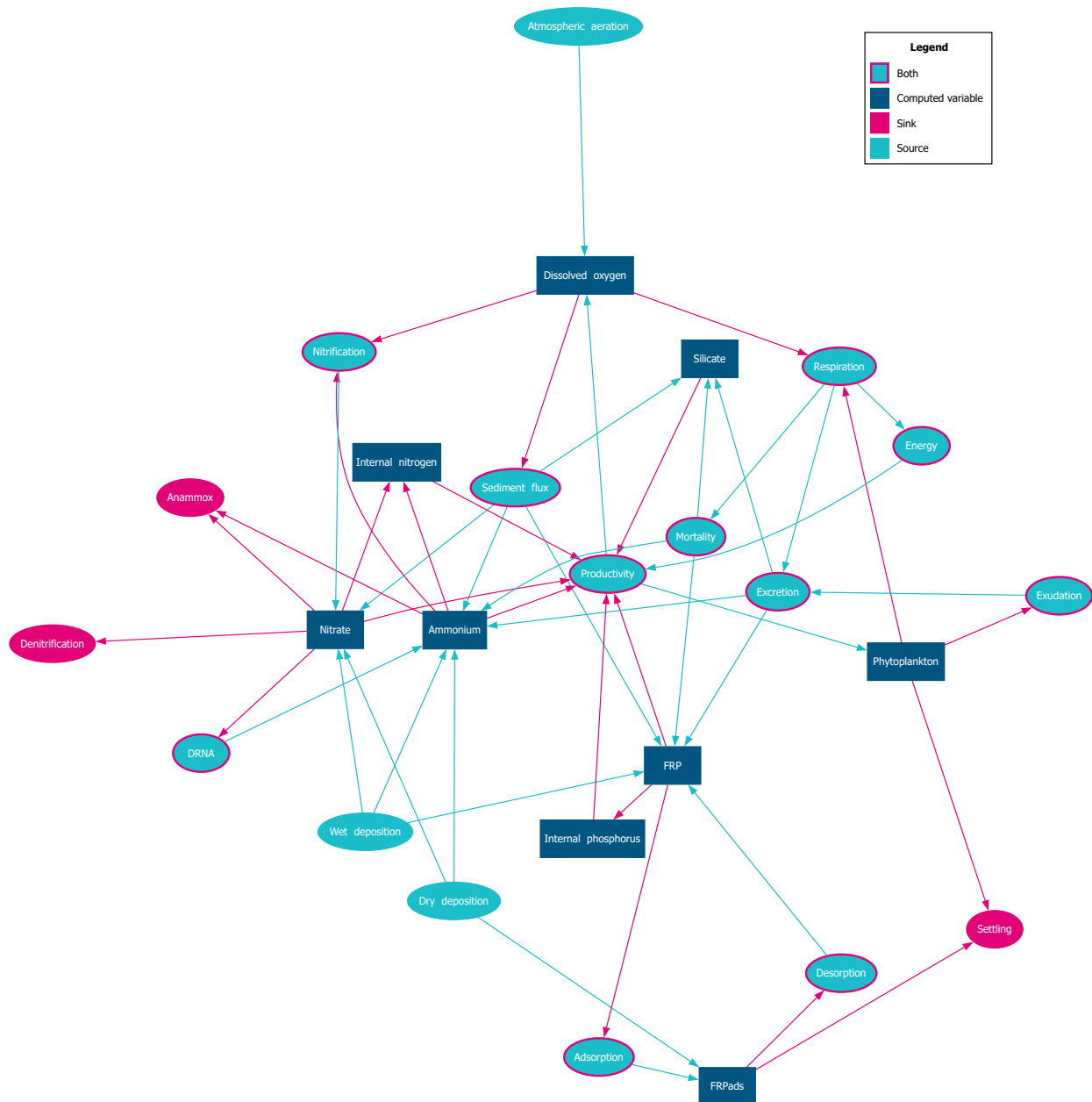


Figure 3.12: Constituent model: Inorganics

3.3 Simulation Class: Organics

3.3.1 Overview

The intent of this simulation class is that it provide a relatively advanced water quality modelling tool. There are many applications for this class. For example it might be used to examine detailed reservoir phytoplankton dynamics or the response of an estuary to both inorganic and organic pollutant loading.

This simulation class includes the oxygen, silicate, inorganic nitrogen, inorganic phosphorus, organic matter, phytoplankton and (optionally) pathogen model classes.

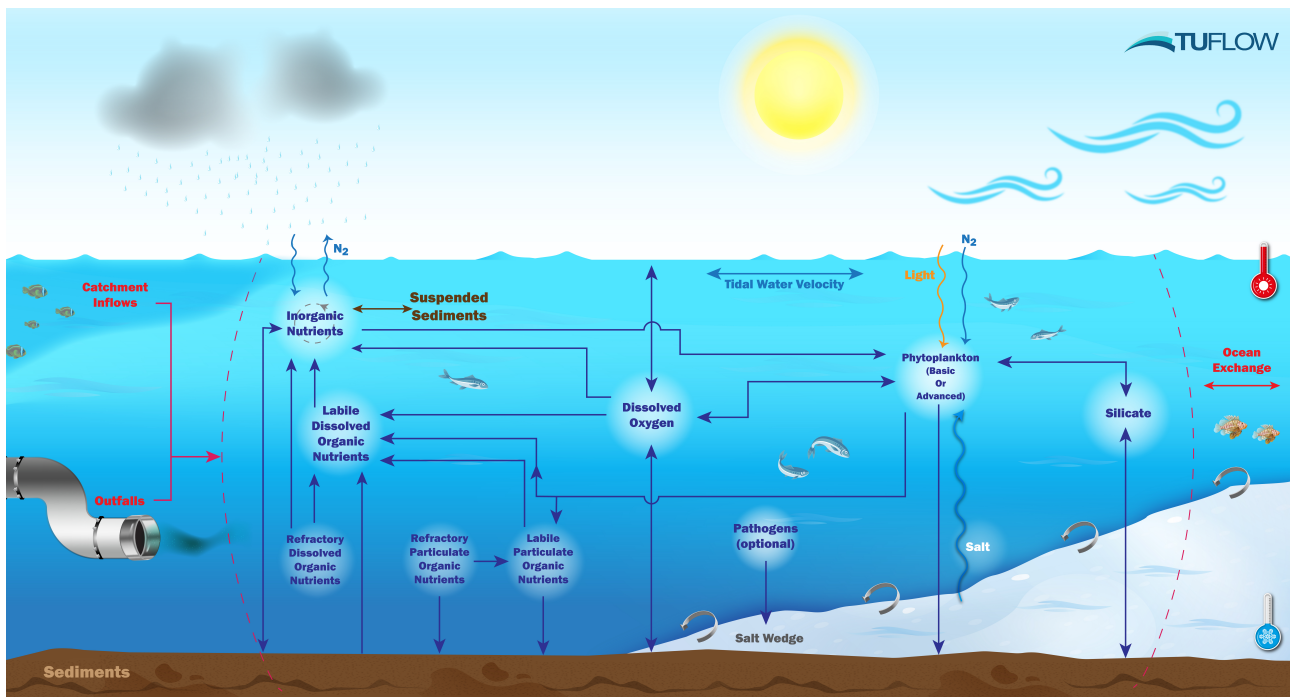


Figure 3.13: Simulation Class: Organics (as an estuarine example)

3.3.2 Model Class: Oxygen

This constituent model class is the same as that described in Section 3.1.2

3.3.3 Model Class: Silicate

This constituent model class is the same as that described in Section 3.2.3

3.3.4 Model Class: Inorganic nitrogen

This constituent model class is the same as that described in Section 3.2.4

3.3.5 Model Class: Inorganic phosphorus

This constituent model class is the same as that described in Section 3.2.5

3.3.6 Model Class: Organic matter

The following constituent models are available to select from within the organic matter model class. The differentiator between constituent models is the exclusion or inclusion of refractory organic matter.

3.3.6.1 Constituent Model: Labile

This organic matter constituent model considers only labile particulate and dissolved organic matter. The constituent model code and associated computed variables, processes and potentially interacting simulated quantities are provided in Figure 3.14 and Table 3.13. Both the Figure and Table (and Table 3.14) make reference to dissolved inorganic carbon (DIC). This is for completeness only because the WQ Module does not currently support simulation of DIC. Doing so is not required in order to deploy either the labile or refractory organic matter constituent model within the WQ Module.

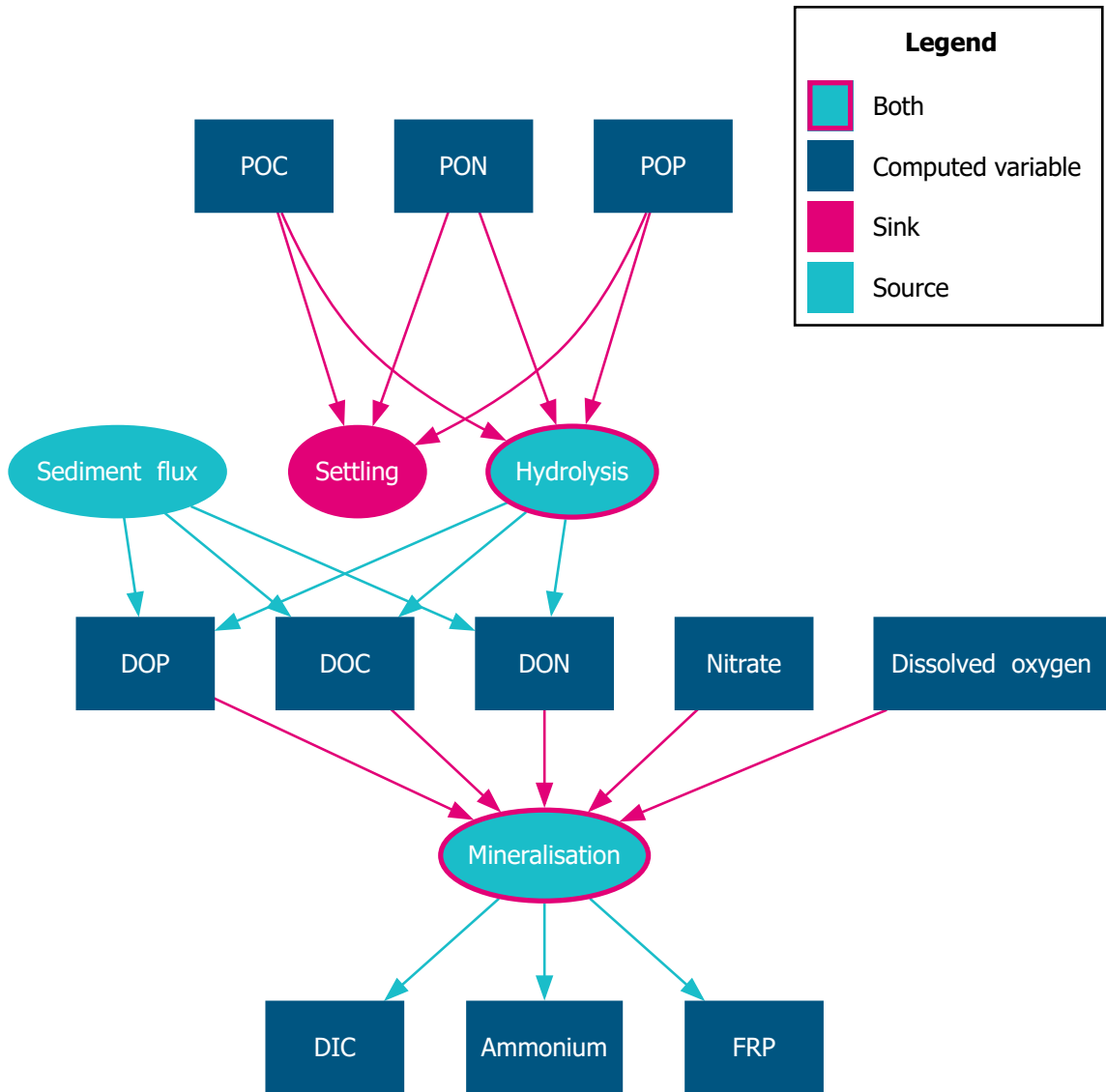


Figure 3.14: Constituent model: Labile

Table 3.13: Constituent model properties - Labile

Computed Variables	Units	Processes	Interacting Quantities
Labile Particulate Organic Carbon	mg C/L or mmol C/m ³	Hydrolysis Settling	<ul style="list-style-type: none">Water temperatureDissolved oxygenSettling model
Labile Particulate Organic Nitrogen	mg N/L or mmol N/m ³	Hydrolysis Settling	<ul style="list-style-type: none">Water temperatureDissolved oxygenSettling model
Labile Particulate Organic Phosphorus	mg P/L or mmol P/m ³	Hydrolysis	<ul style="list-style-type: none">Water temperatureDissolved oxygen

Table 3.13: Constituent model properties - Labile

Computed Variables	Units	Processes	Interacting Quantities
Labile Dissolved Organic Carbon	mg C/L or mmol C/m ³	Settling	• Settling model
		Sediment Flux	• Water temperature • Dissolved oxygen • Sediment properties
		Hydrolysis	• Water temperature • Dissolved oxygen • POC
Labile Dissolved Organic Nitrogen	mg N/L or mmol N/m ³	Mineralisation	• Water temperature • Dissolved oxygen • Nitrate
		Sediment Flux	• Water temperature • Dissolved oxygen • Sediment properties
		Hydrolysis	• Water temperature • Dissolved oxygen • PON
Labile Dissolved Organic Phosphorus	mg P/L or mmol P/m ³	Mineralisation	• Water temperature • Dissolved oxygen • Nitrate
		Sediment Flux	• Water temperature • Dissolved oxygen • Sediment properties
		Hydrolysis	• Water temperature • Dissolved oxygen • POP
		Mineralisation	• Water temperature • Dissolved oxygen • Nitrate

The four processes that govern (labile) organic matter behaviour in this constituent model are:

- Sediment flux
- Hydrolysis (the conversion of particulate organics to dissolved organics)
- Mineralisation (the conversion of dissolved organics to inorganics), and
- Settling, of only particulate organics

A range of rate constants can be specified to control these processes, or the defaults used. By design, the library default rates are set to zero so as to render all processes initially inactive. Specification of non-zero rates activates these processes.

Simulation of labile organic dynamics in the organics simulation class directly modifies the concentrations of other computed variables. These are listed in Table 3.14.

Table 3.14: Complementary lower order computed variables - Labile

Computed Variables	Units	Processes	Interacting Quantities
Dissolved Oxygen	mg/L or mmol/m ³	Mineralisation	• Water temperature • Dissolved oxygen • DOC • DON • DOP

Table 3.14: Complementary lower order computed variables - Labile

Computed Variables	Units	Processes	Interacting Quantities
Nitrate	mg/L or mmol/m ³	Mineralisation	<ul style="list-style-type: none"> • Water temperature • Dissolved oxygen • Nitrate • DOC • DON • DOP
Ammonium	mg/L or mmol/m ³	Mineralisation	<ul style="list-style-type: none"> • Water temperature • Dissolved oxygen • Nitrate • DON
FRP	mg/L or mmol/m ³	Mineralisation	<ul style="list-style-type: none"> • Water temperature • Dissolved oxygen • Nitrate • DOP
DIC	mg/L or mmol/m ³	Mineralisation	<ul style="list-style-type: none"> • Water temperature • Dissolved oxygen • Nitrate • DOC

3.3.6.2 Constituent Model: Refractory

This organic matter constituent model considers both labile and refractory particulate and dissolved organic matter. The constituent model code and associated computed variables, processes and potentially interacting simulated quantities are provided in Figure 3.15 and Table 3.15. Both the Figure and Table (and Table 3.16) make reference to dissolved inorganic carbon (DIC). This is for completeness only because the WQ Module does not currently support simulation of DIC. Doing so is not required in order to deploy either the labile or refractory organic matter constituent model within the WQ Module.

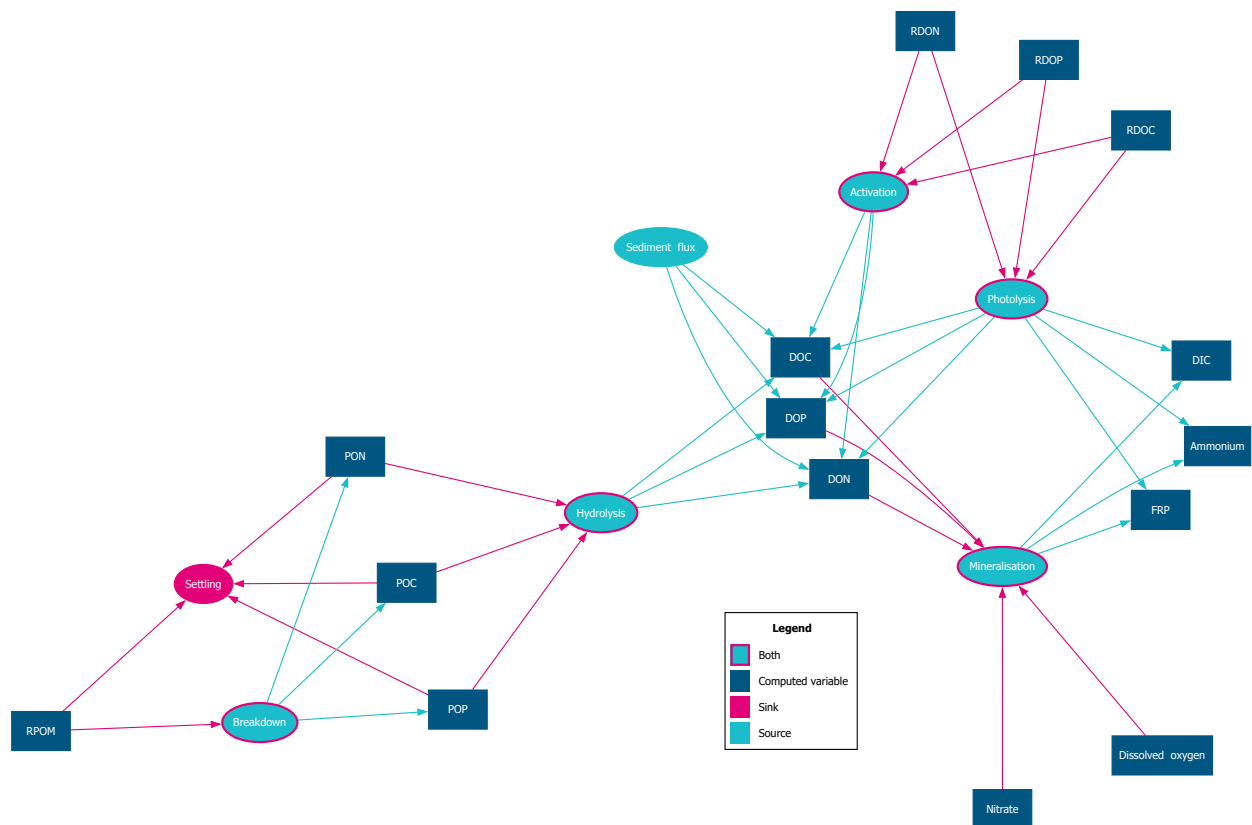


Figure 3.15: Constituent model: Refractory

Table 3.15: Constituent model properties - Refractory

Computed Variables	Units	Processes	Interacting Quantities
Labile Particulate Organic Carbon	mg C/L or mmol C/m ³	Hydrolysis Settling Breakdown	<ul style="list-style-type: none"> Water temperature Dissolved oxygen Settling model Water temperature Dissolved oxygen RPOM
Labile Particulate Organic Nitrogen	mg N/L or mmol N/m ³	Hydrolysis Settling Breakdown	<ul style="list-style-type: none"> Water temperature Dissolved oxygen Settling model Water temperature Dissolved oxygen RPOM
Labile Particulate Organic Phosphorus	mg P/L or mmol P/m ³	Hydrolysis Settling Breakdown	<ul style="list-style-type: none"> Water temperature Dissolved oxygen Settling model Water temperature Dissolved oxygen RPOM

Table 3.15: Constituent model properties - Refractory

Computed Variables	Units	Processes	Interacting Quantities
Labile Dissolved Organic Carbon	mg C/L or mmol C/m ³	Sediment Flux	<ul style="list-style-type: none"> Water temperature Dissolved oxygen Sediment properties
		Hydrolysis	<ul style="list-style-type: none"> Water temperature Dissolved oxygen POC
		Mineralisation	<ul style="list-style-type: none"> Water temperature Dissolved oxygen Nitrate
		Activation	<ul style="list-style-type: none"> Water temperature Dissolved oxygen RDOC
		Photolysis	<ul style="list-style-type: none"> Radiation RDOC
Labile Dissolved Organic Nitrogen	mg N/L or mmol N/m ³	Sediment Flux	<ul style="list-style-type: none"> Water temperature Dissolved oxygen Sediment properties
		Hydrolysis	<ul style="list-style-type: none"> Water temperature Dissolved oxygen PON
		Mineralisation	<ul style="list-style-type: none"> Water temperature Dissolved oxygen Nitrate
		Activation	<ul style="list-style-type: none"> Water temperature Dissolved oxygen RDON
		Photolysis	<ul style="list-style-type: none"> Radiation RDON
Labile Dissolved Organic Phosphorus	mg P/L or mmol P/m ³	Sediment Flux	<ul style="list-style-type: none"> Water temperature Dissolved oxygen Sediment properties
		Hydrolysis	<ul style="list-style-type: none"> Water temperature Dissolved oxygen POP
		Mineralisation	<ul style="list-style-type: none"> Water temperature Dissolved oxygen Nitrate
		Activation	<ul style="list-style-type: none"> Water temperature Dissolved oxygen RDOP
		Photolysis	<ul style="list-style-type: none"> Radiation RDOP
Refractory Particulate Organic Carbon	mg C/L or mmol C/m ³	Settling	<ul style="list-style-type: none"> Settling model
		Breakdown	<ul style="list-style-type: none"> Water temperature Dissolved oxygen
Refractory Dissolved Organic Carbon	mg C/L or mmol C/m ³	Activation	<ul style="list-style-type: none"> Water temperature Dissolved oxygen
		Photolysis	<ul style="list-style-type: none"> Radiation RDOC

Table 3.15: Constituent model properties - Refractory

Computed Variables	Units	Processes	Interacting Quantities
Refractory Dissolved Organic Nitrogen	mg N/L or mmol N/m ³	Activation Photolysis	<ul style="list-style-type: none"> • Water temperature • Dissolved oxygen • Radiation • RDOC • RDON
Refractory Dissolved Organic Phosphorus	mg N/L or mmol N/m ³	Activation Photolysis	<ul style="list-style-type: none"> • Water temperature • Dissolved oxygen • Radiation • DOC • RDOC • RDOP

The processes that govern (labile and refractory) organic matter behaviour in this constituent model are:

- Sediment flux
- Hydrolysis (the conversion of particulate organics to dissolved organics)
- Mineralisation (the conversion of dissolved organics to inorganics)
- Breakdown (the conversion of refractory particulate organic matter to labile particulate organic matter)
- Photolysis (the conversion of refractory dissolved organic matter to labile dissolved organic matter and corresponding inorganics)
- Activation (the conversion of refractory dissolved to labile dissolved organic matter)
- Settling, of only particulate organics

A range of rate constants can be specified to control these processes, or the defaults used. By design, the library default rates are set to zero so as to render all processes initially inactive. Specification of non-zero rates activates these processes.

Simulation of labile and refractory organic dynamics in the organics simulation class directly modifies the concentrations of other computed variables. These are listed in Table 3.16.

Table 3.16: Complementary lower order computed variables - Refractory

Computed Variables	Units	Processes	Interacting Quantities
Dissolved Oxygen	mg/L or mmol/m ³	Mineralisation	<ul style="list-style-type: none"> • Water temperature • Dissolved oxygen
Nitrate	mg/L or mmol/m ³	Mineralisation	<ul style="list-style-type: none"> • Water temperature • Dissolved oxygen • Nitrate
Ammonium	mg/L or mmol/m ³	Mineralisation Photolysis	<ul style="list-style-type: none"> • Water temperature • Dissolved oxygen • Nitrate • Radiation • RDON
FRP	mg/L or mmol/m ³	Mineralisation Photolysis	<ul style="list-style-type: none"> • Water temperature • Dissolved oxygen • Nitrate • Radiation • RDOP
DIC		Mineralisation	<ul style="list-style-type: none"> • Water temperature • Dissolved oxygen • Nitrate

Table 3.16: Complementary lower order computed variables - Refractory

Computed Variables	Units	Processes	Interacting Quantities
		Photolysis	<ul style="list-style-type: none"> • Radiation • RDOC

3.3.7 Model Class: Phytoplankton

This constituent model class is the same as that described in Section 3.2.6, except that in the current constituent model class, phytoplanktonic losses are to labile organic computed variables rather than inorganic nutrients. These processes and interactions are described below.

3.3.7.1 Constituent Model: Basic

As per Section 3.2.6.1, this phytoplankton constituent model assumes that the ratios of both internal nitrogen and phosphorus concentrations to internal chlorophyll *a* (or carbon) concentration are fixed. These internal nutrients are not simulated explicitly, but increase and decrease proportionately with increasing and decreasing carbonaceous biomass, according to the specified (or default) nitrogen-chlorophyll *a* and phosphorus-chlorophyll *a* (or their carbon equivalents) ratios. Carbonaceous biomass is simulated dynamically and is the measure of phytoplankton concentration. Internal nutrient concentrations are not required to be specified as initial or boundary conditions, and are not treated as computed variables.

The constituent model code and associated computed variables, processes and potentially interacting simulated quantities are provided in Figure 3.16 and Table 3.17. Silicate interactions only apply if phytoplankton is set to uptake silicate via specification of silicate limitation function parameters (Section 4.7.3.5.1). The configuration for phytoplankton simulation presented below applies only to the organics simulation class. A different, and simpler, configuration applies when phytoplankton is simulated using this basic constituent model in the inorganics simulation class. That simplified configuration is described in Section 3.2.6.1.

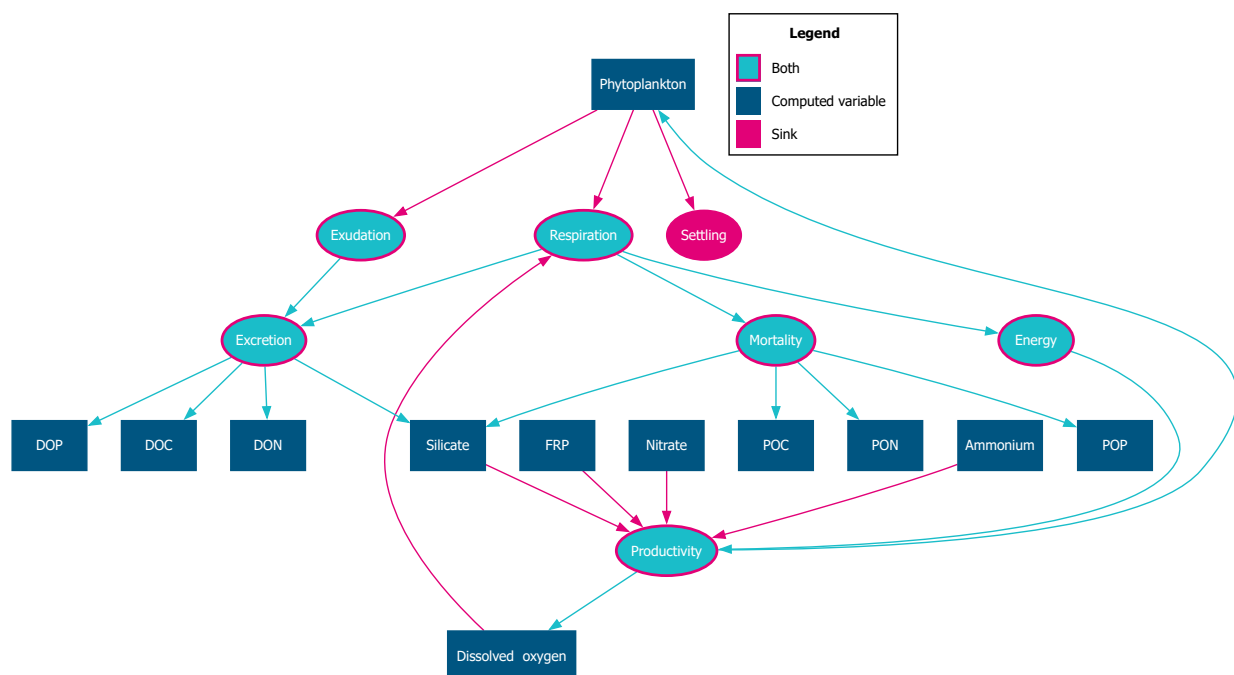


Figure 3.16: Constituent model: Basic

Table 3.17: Constituent model properties - Basic

Computed Variables	Units	Processes	Interacting Quantities
Phytoplankton	$\mu\text{g Chl } a/\text{L}$ or $\text{mmol C}/\text{m}^3$	Primary Productivity	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Dissolved oxygen • Ammonium • Nitrate • FRP • Silicate (if activated)
		Respiration	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Dissolved oxygen
		Excretion	<ul style="list-style-type: none"> • DOC • DON • DOP • Silicate (if activated)
		Mortality	<ul style="list-style-type: none"> • POC • PON • POP • Silicate (if activated)
		Settling	<ul style="list-style-type: none"> • Settling model • Cell density

The three processes that govern phytoplankton behaviour are:

- Primary productivity (the photosynthetic conversion of light and carbon to stored energy and oxygen, also referred to as growth)
- Respiration (the expenditure of stored energy and oxygen), and
- Settling

A range of light, temperature, salinity, nitrogen, phosphorus and silicate limitation functions can be parameterised and applied in various combinations to the first two processes above, and a range of settling models are available to tailor the third. By design, the associated library default rates are set to zero so as to render all processes initially inactive. Specification of non-zero rates activates these processes.

The distinguishing property of this phytoplankton constituent model is that internal (phytoplankton cell) nutrient concentrations are considered to be fixed proportions of cell chlorophyll *a* (or carbon) concentrations. They are therefore not treated as computed variables, but rather as multiples of phytoplankton chlorophyll *a* (or carbon) (which is treated as a computed variable). The key implication of this is the method of calculation of the nitrogen and phosphorus uptake and limitation functions applied to primary productivity. These calculations depend only on ambient (i.e. external to a phytoplankton cell) water column nitrogen and phosphorus concentrations.

Simulation of phytoplankton dynamics in the organics simulation class directly modifies the concentrations of a range of other computed variables. These are listed in Table 3.18. Silicate interactions only apply if phytoplankton is set to uptake silicate.

Table 3.18: Complementary lower order computed variables - Basic

Computed Variables	Units	Processes	Interacting Quantities
Dissolved Oxygen	mg/L or mmol/m ³	Primary Productivity	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Ammonium • Nitrate • FRP • Silicate (if activated)
		Respiration	<ul style="list-style-type: none"> • Water temperature • Salinity • Light
Ammonium	mg/L or mmol/m ³	Primary Productivity	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Nitrate • FRP • Silicate (if activated)
Nitrate	mg/L or mmol/m ³	Primary Productivity	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Ammonium • FRP • Silicate (if activated)
FRP	mg/L or mmol/m ³	Primary Productivity	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Nitrate • Ammonium • Silicate (if activated)
Silicate (if activated)	mg/L or mmol/m ³	Primary Productivity	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Nitrate • Ammonium • FRP
		Excretion	<ul style="list-style-type: none"> • DOC • DON • DOP
		Mortality	<ul style="list-style-type: none"> • POC • PON • POP
Labile Particulate Organic Carbon	mg/L or mmol/m ³	Mortality	<ul style="list-style-type: none"> • PON • POP • Silicate (if activated)
Labile Particulate Organic Nitrogen	mg/L or mmol/m ³	Mortality	<ul style="list-style-type: none"> • POC • POP • Silicate (if activated)
Labile Particulate Organic Phosphorus	mg/L or mmol/m ³	Mortality	<ul style="list-style-type: none"> • POC • PON • Silicate (if activated)

Table 3.18: Complementary lower order computed variables - Basic

Computed Variables	Units	Processes	Interacting Quantities
Labile Dissolved Organic Carbon	mg/L or mmol/m ³	Excretion	<ul style="list-style-type: none"> • DON • DOP • Silicate (if activated)
Labile Dissolved Organic Nitrogen	mg/L or mmol/m ³	Excretion	<ul style="list-style-type: none"> • DOC • DOP • Silicate (if activated)
Labile Dissolved Organic Phosphorus	mg/L or mmol/m ³	Excretion	<ul style="list-style-type: none"> • DOC • DON • Silicate (if activated)

3.3.7.2 Constituent Model: Advanced

As per Section 3.2.6.2, this phytoplankton constituent model directly simulates internal (phytoplankton cell) nitrogen and phosphorus concentrations. These are allowed to vary between upper and lower limits, expressed as ratios to chlorophyll *a* (or carbon) concentrations. Internal nutrient concentrations (not as ratios) are required to be specified as initial and boundary conditions, and are treated as computed variables.

The constituent model code and associated variables, processes and potentially interacting simulated quantities are provided in Figure 3.17 and Table 3.19. Silicate interactions only apply if phytoplankton is set to uptake silicate. The configuration for phytoplankton simulation presented below applies only to the organics simulation class. A different, and simplified, configuration applies when phytoplankton is simulated using this advanced constituent model in the inorganics simulation class. That configuration is described in Section 3.2.6.2.

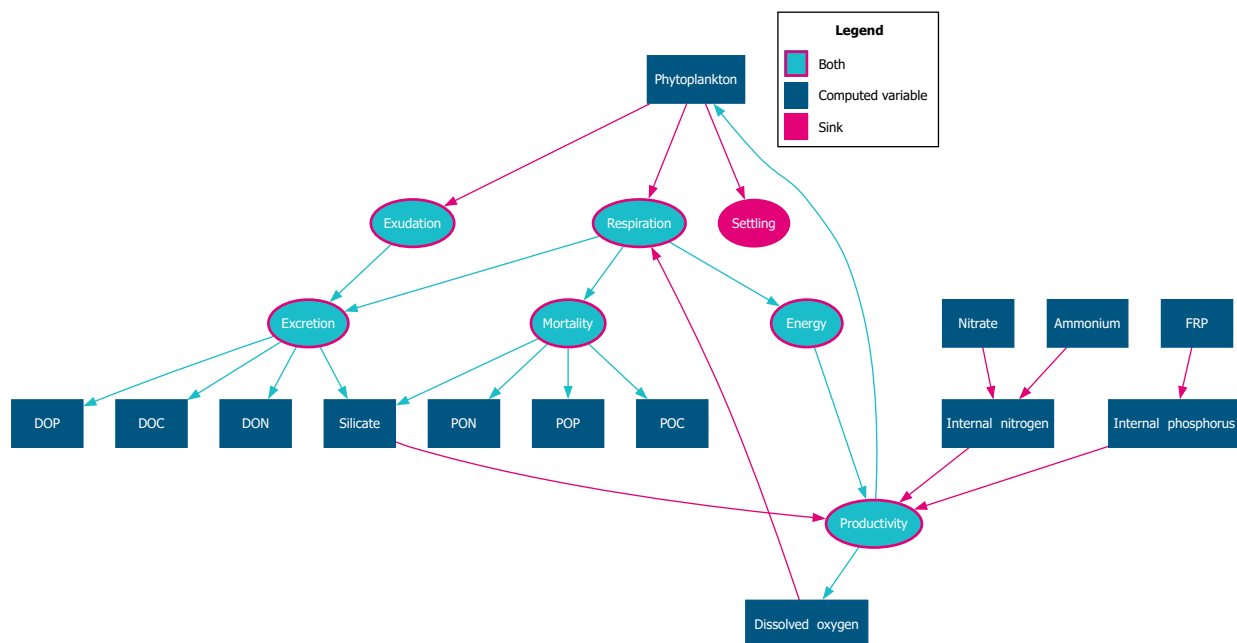
**Figure 3.17: Constituent model: Advanced**

Table 3.19: Constituent model properties - Advanced

Computed Variables	Units	Processes	Interacting Quantities
Phytoplankton	$\mu\text{g Chl } a/\text{L}$ or $\text{mmol C}/\text{m}^3$	Primary Productivity	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Dissolved oxygen • Ammonium • Nitrate • FRP • Internal nitrogen • Internal phosphorus • Silicate (if activated)
		Respiration	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Dissolved oxygen • Internal nitrogen • Internal phosphorus
		Excretion	<ul style="list-style-type: none"> • DOC • DON • DOP • Internal nitrogen • Internal phosphorus • Silicate (if activated)
		Mortality	<ul style="list-style-type: none"> • POC • PON • POP • Internal nitrogen • Internal phosphorus • Silicate (if activated)
		Settling	<ul style="list-style-type: none"> • Settling model • Cell density • Internal nitrogen • Internal phosphorus
Internal Nitrogen	$\text{mg N}/\text{L}$ or $\text{mmol N}/\text{m}^3$	Primary Productivity	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Dissolved oxygen • Ammonium • Nitrate • FRP • Internal phosphorus • Silicate (if activated)
		Uptake	<ul style="list-style-type: none"> • Water temperature • Ammonium • Nitrate • FRP • Internal phosphorus • Silicate (if activated)
		Respiration	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Dissolved oxygen • Internal phosphorus

Table 3.19: Constituent model properties - Advanced

Computed Variables	Units	Processes	Interacting Quantities
Internal Phosphorus	mg P/L or mmol P/m ³	Excretion	<ul style="list-style-type: none"> • DOC • DON • DOP • Internal phosphorus • Silicate (if activated)
		Mortality	<ul style="list-style-type: none"> • POC • PON • POP • Internal phosphorus • Silicate (if activated)
		Settling	<ul style="list-style-type: none"> • Settling model • Cell density • Internal phosphorus
		Primary Productivity	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Dissolved oxygen • Ammonium • Nitrate • FRP • Internal nitrogen • Silicate (if activated)
		Uptake	<ul style="list-style-type: none"> • Water temperature • Ammonium • Nitrate • FRP • Internal nitrogen • Silicate (if activated)
		Respiration	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Dissolved oxygen • Internal nitrogen
		Excretion	<ul style="list-style-type: none"> • DOC • DON • DOP • Internal nitrogen • Silicate (if activated)
		Mortality	<ul style="list-style-type: none"> • POC • PON • POP • Internal nitrogen • Silicate (if activated)
		Settling	<ul style="list-style-type: none"> • Settling model • Cell density • Internal nitrogen

The three processes that govern phytoplankton behaviour are:

- Primary productivity (the photosynthetic conversion of light and carbon to stored energy and oxygen, also referred to as growth)

- Respiration (the expenditure of stored energy and oxygen), and
- Settling

A range of light, temperature, salinity, nitrogen, phosphorus and silicate limitation functions can be parameterised and applied in various combinations to the first two processes above, and a range of settling models are available to tailor the third. By design, the associated library default rates are set to zero so as to render all processes initially inactive. Specification of non-zero rates activates these processes.

The distinguishing property of this phytoplankton constituent model is that internal (phytoplankton cell) nutrient concentrations are simulated directly. They are therefore treated as computed variables. The key implication of this is the method of calculation of the nitrogen and phosphorus uptake and limitation functions applied to primary productivity. These calculations depend on both internal nutrient stores and ambient (i.e. external to a phytoplankton cell) water column nitrogen and phosphorus concentrations.

Simulation of phytoplankton dynamics in the organics simulation class directly modifies the concentrations of a range of other computed variables. These are listed in Table 3.20. Silicate interactions only apply if phytoplankton is set to uptake silicate.

Table 3.20: Complementary lower order computed variables - Advanced

Computed Variables	Units	Processes	Interacting Quantities
Dissolved Oxygen	mg/L or mmol/m ³	Primary Productivity Respiration	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Ammonium • Nitrate • FRP • Internal nitrogen • Internal phosphorus • Silicate (if activated) • Water temperature • Salinity • Light
Ammonium	mg/L or mmol/m ³	Primary Productivity	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Nitrate • Internal nitrogen • Internal phosphorus • FRP • Silicate (if activated)
Nitrate	mg/L or mmol/m ³	Primary Productivity	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Ammonium • Internal nitrogen • Internal phosphorus • FRP • Silicate (if activated)
FRP	mg/L or mmol/m ³	Primary Productivity	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Nitrate • Ammonium • Internal phosphorus • Silicate (if activated)

Table 3.20: Complementary lower order computed variables - Advanced

Computed Variables	Units	Processes	Interacting Quantities
Silicate (if activated)	mg/L or mmol/m ³	Primary Productivity Excretion Mortality	<ul style="list-style-type: none"> • Water temperature • Salinity • Light • Nitrate • Ammonium • FRP • Internal nitrogen • Internal phosphorus • DOC • DON • DOP • Internal nitrogen • Internal phosphorus • POC • PON • POP • Internal nitrogen • Internal phosphorus
Labile Particulate Organic Carbon	mg/L or mmol/m ³	Mortality	<ul style="list-style-type: none"> • PON • POP • Internal nitrogen • Internal phosphorus • Silicate (if activated)
Labile Particulate Organic Nitrogen	mg/L or mmol/m ³	Mortality	<ul style="list-style-type: none"> • POC • POP • Internal nitrogen • Internal phosphorus • Silicate (if activated)
Labile Particulate Organic Phosphorus	mg/L or mmol/m ³	Mortality	<ul style="list-style-type: none"> • POC • PON • Internal nitrogen • Internal phosphorus • Silicate (if activated)
Labile Dissolved Organic Carbon	mg/L or mmol/m ³	Excretion	<ul style="list-style-type: none"> • DON • DOP • Internal nitrogen • Internal phosphorus • Silicate (if activated)
Labile Dissolved Organic Nitrogen	mg/L or mmol/m ³	Excretion	<ul style="list-style-type: none"> • DOC • DOP • Internal nitrogen • Internal phosphorus • Silicate (if activated)
Labile Dissolved Organic Phosphorus	mg/L or mmol/m ³	Excretion	<ul style="list-style-type: none"> • DOC • DON • Internal nitrogen • Internal phosphorus • Silicate (if activated)

3.3.8 Model Class: Pathogens (optional)

This model class is the same as that described in Section 3.1.3.

3.3.9 Computed variables

The relationships between all available computed variables and processes in this simulation class are presented in Figure 3.18. Depending on the constituent model classes deployed, not all of the computed variables and processes shown in the figure will necessarily be active. All network link labels have been removed (other than denoting the relevant phytoplankton model), and optional non-interacting model classes (e.g. pathogens) omitted, for clarity.

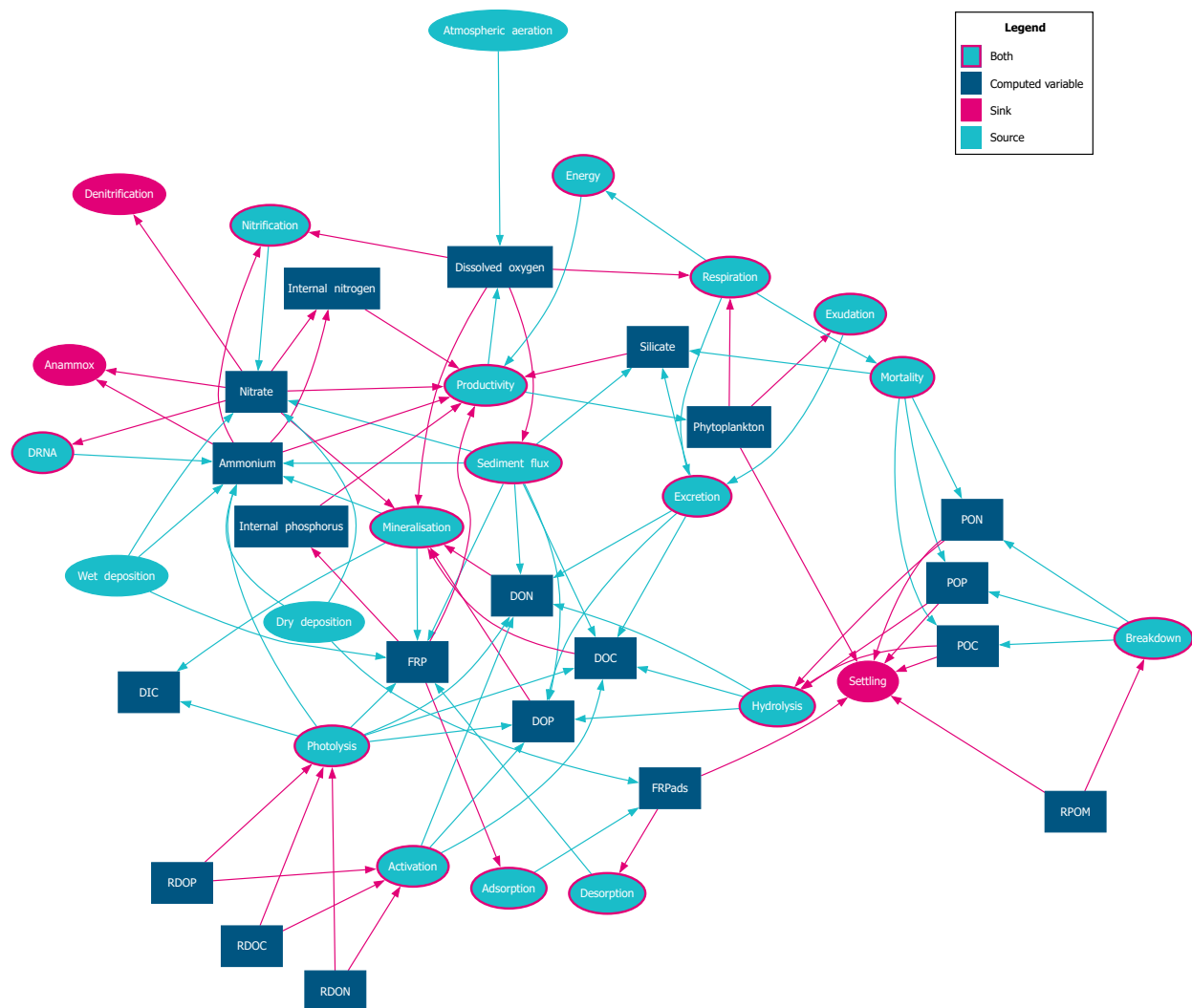


Figure 3.18: Simulation class: Organics

4 Simulation Construction

4.1 Context

Previous sections have presented the architecture and water quality processes available within the WQ Module. This section describes the construction of a TUFLOW simulation with the WQ Module activated. This includes descriptions of all commands, with hyperlinks to the Appendices where commands and explanations are listed. TUFLOW FV is the hydrodynamic model used in all descriptions that follow.

Optional model classes (such as pathogens) and their construction are first described in the simplest simulation class for which they can be deployed. Commentary on the ordering of optional constituents is provided in subsequent sections only where needed.

4.2 Units

The WQ Module allows for simulation construction in one of two unit systems (see Section 4.5.1):

- A milligrams per litre system (which includes micrograms per litre for phytoplankton) that aligns with typical units of laboratory reporting, and
- A millimoles per cubic metre system

A single units system must be adopted for a WQ Module simulation, and unit systems cannot be mixed within a simulation. This specification has implications for at least the setting of numerical values for:

- Initial conditions
- Boundary conditions
- Computed variable parameters

When the milligrams per litre system is used, the WQ Module executes internal conversions between milligrams and millimoles, because millimoles are the units expected by the core water quality calculation routines. This conversion follows the form:

$$n = \frac{m}{M} \quad (4.1)$$

where n is millimoles (mmol), m is mass (mg) and M is molar weight (mg/mmol). A similar concept applies to concentration and flux quantities. As such, the WQ Module assigns values to M in converting from milligrams to millimoles, i.e. from user specified milligram initial conditions, boundary conditions and computed variable parameters, to the equivalent millimole quantities. The complete list of values of M for all simulated constituents is provided in Appendix O. The two possibilities for units for each parameter are provided in Appendix A, where relevant.

As an example, if a user specifies the milligrams per litre units system (or allows the same default to be set) and sets `FRP Flux == 3.1` in a materials block, then this value of 3.1 is assumed to be mg/m²/day. Consistent with typical laboratory reporting conventions (see below), this mass flux is taken to be that of elemental phosphorus P , not that of the phosphate molecule PO_4^{3-} . This would mean (using Appendix O and Equation 4.1) that the equivalent millimole rate would be computed as:

$$n = \frac{3.1}{31} = 0.1 \text{ mmol/m}^2/\text{day of P} \quad (4.2)$$

Given the above, users opting to construct WQ Module simulations in the milligrams units system need to clearly understand what is being reported in:

- Field and/or laboratory measurements, and
- Other numerical model predictions that may be used as WQ Module boundary conditions (such as catchment pollutant export models)

In the case of laboratory nutrient measurements, it is conventional to report concentrations of the typical quantities used by the WQ Module as silicate-Si, ammonium-N, nitrate-N, FRP-P, organic-C, organic-N, and organic-P. Whilst these quantities might be referred to informally as (for example) “nitrate concentrations”, the reported number is most commonly the concentration of elemental nitrogen contained within nitrate. To be clear, if a nitrate-N concentration is reported by a laboratory to be 3.5 mg/L, this means that in every litre of water, there are 3.5 milligrams of elemental nitrogen contained within nitrate molecules. Given the molar masses of elemental nitrogen and nitrate, this 3.5 milligrams of elemental N means that there are 15.5 milligrams of nitrate molecules ($15.5 = 3.5 \times 62/14$) in the same litre of water. In this example, the concentration with which the WQ Module expects to be provided is 3.5 mg/L, not 15.5 mg/L.

The use of other model data to force WQ Module boundary conditions is also interpreted in this way. For example, a catchment model might report that an inflow to the WQ Module at an upstream riverine boundary condition has a “total nitrogen” concentration of 10.0 mg/L, and a user may have then speciated this to nitrate by applying a multiplicative factor of 0.15. If this resulting nitrate concentration of 1.5 mg/L is applied to the WQ Module as a boundary condition, it must be a concentration of elemental nitrogen within nitrate, which is consistent with what would be reported by a laboratory. This means that the user must be sure that the “total nitrogen” reported by the catchment model is in fact an elemental nitrogen concentration.

If users elect to construct WQ Module simulations in units of millimoles, then no internal WQ Module conversions take place, and the nature of the quantity (molecular or elemental) being specified is not relevant. For example, the user could specify millimoles units and `FRP Flux == 0.1`. This could be interpreted as a mmol/m²/day rate of either the PO_4^{3-} molecule, or just phosphorus *P*. This is because in one millimole of PO_4^{3-} , there is also one millimole of elemental *P*. The same one to one relationship holds for all other WQ Module relevant computed quantities (see Appendix O), other than oxygen which is treated as a diatomic molecule.

4.3 General arrangement

A water quality simulation is set up and executed under the umbrella of a TUFLOW FV control file (Figure 4.1, with other optional modules shown for illustrative purposes). That is:

- The TUFLOW FV control file (*.fvc) file remains the central file that initiates and coordinates an overall simulation. This mirrors the way in which other TUFLOW FV modules, such as the ST Module and PT Module, are activated and executed
- The TUFLOW FV control file contains a path to a separate WQ Module control file (*.fwq) that in turn contains all the commands required to configure a WQ Module simulation

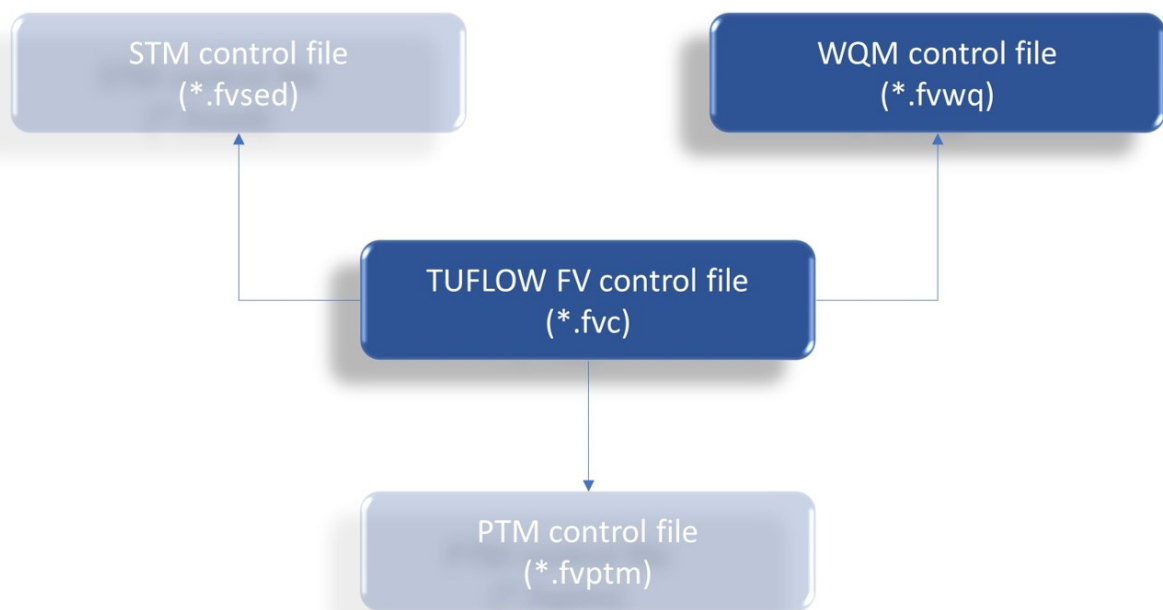


Figure 4.1: Simulation Coordination

TUFLOW FV and WQ Module control file commands are presented following.

4.4 TUFLOW FV control file commands

A TUFLOW FV simulation is executed as described in the TUFLOW FV user manual. If the WQ Module is to be activated in a simulation then the following commands are to be included.

4.4.1 WQ Module activation

Activation of the WQ Module is affected by specification of the following mandatory command in the TUFLOW control file:

```
Water Quality Model == TUFLOW
```

Following this activation, TUFLOW FV will look for the specification of the name of the separate WQ Module control file via the following mandatory command:

```
Water Quality Control File == <_water quality control file name_>.fvwq
```

This *.fvwq is separate to the *.fvc and contains user specified information that describes the configuration of the water quality simulation. If the *.fvwq is located in the same directory as the *.fvc, then this filename specification needs no associated path. It is recommended however that the *.fvwq be located in a directory separate to the *.fvc so that log and other related water quality specific files can be easily curated. If this approach is adopted, the following additional *.fvc command is required, noting that the folder path is specified as relative to the folder in which the *.fvc resides:

```
Water Quality Model Directory == <_relative path to WQ directory_>\
```

This command must terminate in a \ character. If this command is issued, then the *.fvwq water quality control file must be located in the directory specified.

In certain circumstances, executing water quality calculations in shallow cells can cause numerical instabilities. To control this behaviour, the WQ Module allows for water quality calculations to be switched off in cells that have depths less than a specified minimum (advection dispersion calculations will however continue to be performed - it is only

the water quality-related non-conservative transformations that are turned off). This minimum depth (in meters) is specified in the TUFLOW FV *.fvc via the command:

```
Cell Water Quality Depth ==  $d_{min-wq}$ 
```

If this command is not issued then the default minimum depth of 0.01m (1cm) is applied.

This command parallels the TUFLOW FV command that controls the execution of hydrodynamic calculations as a function of water depth:

```
Cell Wet/Dry Depths == Cell Dry Depth (m), Cell Wet Depth (m)
```

In this TUFLOW FV command:

- The cell dry depth value (default = 1.0e-06 m) corresponds to the water depth below which a cell is dropped completely from hydrodynamic (TUFLOW FV) computations (subject to the status of surrounding cells) and is therefore considered to be 'dry'. Cells that have dried in a given time step are given a stat value of 0 in all TUFLOW FV results files, so this stat field acts as a mask to determine which cells are wet and dry when using post processing tools and or scripts. Dry cells are not contoured in QGIS or SMS when viewed, but appear as transparent. If set to a negative value the cell dry depth is set to zero.
- The cell wet depth value (default = 1.0e-02 m) corresponds to the water depth below which a cell's momentum is set to zero in order to avoid unphysical velocities at very low depths. The cell is not considered to be dry and therefore has a stat value of -1. If this value is less than or equal to the cell dry depth, it is set to the cell dry depth.

Given this, it is therefore recommended that across these commands and/or defaults, a user ensures that the following holds (as it does for the default values noted above):

$$\text{cell dry depth} < \text{cell wet depth} < \text{cell water quality depth} \quad (4.3)$$

If, for example, cell water quality depth is set to a value less than cell dry depth, then water quality calculations will be attempted on cells that TUFLOW FV considers to be dry, which is to be avoided. If a situation arose where it was absolutely necessary, then cell water quality depth could be set to a value less than cell wet depth (but still greater than cell dry depth), but this is not recommended. To summarise, and if the recommended relative magnitudes of depths presented in Equation 4.3 is adopted, then the following applies:

- water depth > cell water quality depth: water quality calculations and momentum calculations performed
- cell water quality depth > water depth > cell wet depth : water quality calculations switched off, momentum calculations performed (advection and dispersion calculations also performed on water quality variables)
- cell wet depth > water depth > cell dry depth: water quality calculations switched off, momentum calculations switched off (advection and dispersion calculations also performed)
- cell dry depth > water depth: no calculations performed - cell is considered dry

To support debugging, water quality calculations can also be turned off completely for all cells and all timesteps by issuing this command in the TUFLOW FV *.fvc:

```
Disable Water Quality Model ==  $B_{disable-wq}$ 
```

and setting $B_{disable-wq} = 1$. Omitting this command, or setting $B_{disable-wq}$ to zero ("0") instead of one ("1"), will activate water quality calculations. If this command is set to one ("1"), then the WQ Module will still initialise are report as such, but when TUFLOW executes, the module will not be called.

Consistent with their specification in the *.fvc, the status of these latter two commands and their arguments are reported in the TUFLOW FV log file, rather than the WQ Module log file.

An example block of these five commands that together activate the WQ Module, point TUFLOW FV to the water quality control file ..\wq\$\Model_000.fvwq and set the minimum depth for executing water quality calculations to 5 centimetres is:

```
Water Quality Model == TUFLOW
Water Quality Model Directory == ..\wq\
Water Quality Control File == ..\Model_000.fvwq
Cell Water Quality Depth == 0.05
Disable Water Quality Model == 0
```

4.4.2 Initial and boundary conditions

In addition to activating the WQ Module and specifying its control file, WQ Module initial and boundary condition information is also set through the TUFLOW FV control file. The processes for doing so are described below. These are followed by discussion of the related matter of constituent ordering within initial and boundary condition specifications.

4.4.2.1 Initial conditions

Water quality initial conditions are specified within or via the TUFLOW FV control file, akin to the manner in which the sediment initial conditions are set on behalf of the sediment transport module. This specification is mandatory.

There are currently a number of ways that water quality initial conditions may be specified. All are affected through TUFLOW FV commands which are described in the TUFLOW FV user manual. If no water quality initial conditions are specified, then a simulation will not execute. The specifications relevant to water quality simulations are described below. The potential limitations of some of these approaches are recognised and will be addressed in future release of the WQ Module.

4.4.2.1.1 Restart files

Restart files are binary files that are generated from previous simulations. These can be used as inputs to initialise water quality simulations, provided that the restart and simulation model geometries, and water quality simulation computed variables and units are identical. A restart file is specified for all simulated quantities (not just water quality) and is controlled through commands described in the TUFLOW FV user manual. The key command is

```
Restart == <_restart file name>.rst
```

Most often, restart files are located in the log directory, but this is not mandatory.

4.4.2.1.2 Globally uniform

Globally uniform (i.e. across all spatial dimensions) initial conditions are set via a command issued from within the TUFLOW FV control file. This is often useful in setting initial conditions for simple small water bodies or at the commencement of a modelling process where initial conditions are set to be placeholders and updated at a later time. The command to do so is:

```
Initial WQ Concentration == Ordered Initial Conditions
```

Each water quality computed variable is set to a single value everywhere. These initial concentrations must be specified in a particular order and this order is described in the following sections for different simulation classes. If the above command is used to set water quality initial conditions, then it must be accompanied by parallel commands that set globally uniform salinity, temperature (and optionally sediment) initial conditions:

```
Initial Temperature == 15.0
Initial Water Level == 1.00
Initial Sediment Concentration == 10.0
Initial Salinity == 3.5
```

Setting a mix of globally uniform and other initial conditions (such as profile, 2D or 3D) is not permitted.

4.4.2.1.3 Globally laterally uniform

Globally laterally uniform initial conditions use an initial profile to set hydrodynamic and water quality computed variable concentrations to be everywhere the same laterally, but to vary vertically. This is often useful in setting initial conditions for deep stationary water bodies such as lakes or reservoirs. The command to do so is:

```
Initial Scalar Profile == <initial condition file name>.csv
```

An example of the form of the text file argument <initial condition file name>.csv for simulating five water quality constituents is:

```
Depth,Sal,temp,sed_1,WQ_1,WQ_2,WQ_3,WQ_4,WQ_5
0.0,2.0,22.0,5.0,8.0,22.0,2.6,1.4,0.5
10.0,2.5,15.0,15.0,5.0,32.0,2.6,1.4,0.2
20.0,3.0,10.0,25.0,0.0,42.0,5.6,5.4,0.1
```


If the above command is used, then it must include profile information that also sets laterally uniform salinity, temperature (and optionally sediment) initial conditions. Setting a mix of laterally uniform and other initial conditions (such as globally uniform, 2D or 3D) is not permitted.

The order of these columns in the argument csv file is not important, but the columns headers are keywords and must be used as shown. For example, the following structure for <initial condition file name>.csv is permitted:

```
Depth,temp,WQ_3,Sal,sed_1,WQ_4,WQ_1,WQ_2,WQ_5
0,22,2.6,2.5,1.4,8,22,0.5
10,15,2.6,2.5,15,1.4,5,32,0.2
20,10,3,3,25,5.4,0,42,0.1
```

Notwithstanding this, it is still considered best practise to develop initial and boundary condition files that have a logically sequential order. Water quality initial conditions headers are labelled “wq_1”, “wq_2” onward, and the match between these header labels and water quality computed variables is set by the computed variable ordering of the simulation class deployed.

4.4.2.1.4 Globally vertically uniform

Globally vertically uniform initial conditions use an initial two dimensional map to set hydrodynamic and water quality computed variable concentrations to be everywhere the same vertically, but to vary laterally. This is often useful in setting initial conditions for shallow water bodies that have horizontal concentration gradients such as small estuaries or urban lakes. The command to do so is:

Initial Condition 2D == <initial condition file name>.csv

An example of the form of the text file argument <initial condition file name>.csv for simulating five water quality constituents is:

```
ID,WL,Sal,temp,sed_1,WQ_1
1,1.0,3.5,15,10.0,8.0
2,1.0,3.5,15,10.0,7.5
3,1.0,3.5,15,10.0,7.0
4,1.0,3.5,15,10.0,6.5
```

If the above command is used, then it must include information that also sets vertically uniform salinity and temperature (and optionally sediment) initial conditions, as well as water level. Setting a mix of vertically uniform and other initial conditions (such as globally uniform, laterally uniform or 3D) is not permitted.

The order of these columns in the argument csv file is not important, but the columns headers are keywords and must be used as shown. For example, the following structure for <initial condition file name>.csv is permitted:

```
ID,WQ_1,WL,sed_1,Sal,temp
1,8.0,1.0,10.0,3.5,15
2,7.5,1.0,10.0,3.5,15
3,7.0,1.0,10.0,3.5,15
4,6.5,1.0,10.0,3.5,15
```

Notwithstanding this, it is still considered best practise to develop initial and boundary condition files that have a logically sequential order. Water quality initial conditions headers are labelled “wq_1”, “wq_2” onward, and the match between these header labels and water quality computed variables is set by the computed variable ordering of the simulation class deployed.

4.4.2.1.5 Globally varying

Globally variable initial conditions use an initial three dimensional map to set hydrodynamic and water quality computed variable concentrations at each 3D cell. This is analogous to using a restart file. The command to do so is:

Initial Condition 3D == <initial condition file name>.csv

An example of the form of the text file argument <initial condition file name>.csv for simulating five water quality constituents is as follows, noting that the “ID” column refers to a three dimensional cell ID, rather than the two dimensional column ID used in the **Initial Condition 2D ==** command.

```
ID,WL,Sal,temp,sed_1,WQ_1
1,1.0,3.5,15,10.0,8.0
2,1.0,3.5,14,10.0,7.5
```

```

3,1.0,3.5,13,10.0,7.0
4,1.0,3.5,12,8.0,6.5
5,1.0,3.5,15,10.0,8.0
6,1.0,3.5,14,10.0,7.4
7,1.0,3.5,13,10.0,7.1
8,1.0,3.5,11,9.0,6.6

```

If the above command is used, then it must include information that also sets globally varying salinity and temperature (and optionally sediment) initial conditions, as well as water level. Setting a mix of vertically uniform and other initial conditions (such as globally uniform, laterally uniform or 2D) is not permitted.

The order of these columns in the argument csv file is not important, but the columns headers are keywords and must be used as shown. For example, the following structure for <initial condition file name>.csv is permitted:

```

ID,WQ_1,WL,sed_1,sal,temp
1,8.0,1.0,10.0,3.5,15
2,7.5,1.0,10.0,3.5,14
3,7.0,1.0,10.0,3.5,13
4,6.5,1.0,8.0,3.5,12
5,8.0,1.0,10.0,3.5,15
6,7.4,1.0,10.0,3.5,14
7,7.1,1.0,10.0,3.5,13
8,6.6,1.0,9.0,3.5,12

```

Notwithstanding this, it is still considered best practise to develop initial and boundary condition files that have a logically sequential order. Water quality initial conditions headers are labelled “wq_1”, “wq_2” onward, and the match between these header labels and water quality computed variables is set by the computed variable ordering of the simulation class deployed.

4.4.2.2 Boundary conditions

Water quality boundary conditions are also specified via the *.fvc file, either directly or via an include statement that points TUFLOW FV to a subsidiary boundary condition control file(s). This specification of water quality variable concentrations is optional, so in early water quality model construction stages this specification can be omitted. Omitted water quality boundary conditions will be set to zero. It is not recommended that this approach be taken beyond initial simulation setup stages, but that it be used only to develop a water quality simulation to the point where it executes without issuing error or unwanted warning messages. At this point, all water quality boundary conditions should be assigned.

All TUFLOW boundary conditions that specify water temperature or salinity will also require specification of the behaviour of simulated water quality variables. Common boundary conditions to which this applies include inflows (e.g. types Q, QC, QN, QG and others) and tidal boundaries (e.g. types WLS). Wave and meteorological boundary conditions do not need specification of water quality conditions.

As for initial conditions, boundary conditions that use columnar data structures (e.g. *.csv files) are interpreted using column headers specified in an expected order within calling TUFLOW FV BC blocks. Further detail and the associated ordering is provided in the following sections (Section 4.6, Section 4.7 and Section 4.8 for simulation classes DO, inorganics and organics, respectively).

4.4.2.3 Ordering

Specification of initial conditions and most boundary conditions presently relies on listing water quality variables in a particular order. This applies in all instances when water quality initial or boundary conditions are provided in columnar or list form, which is most frequently in text file format. This is conceptually similar to the manner in which TUFLOW FV also relies on ordering of its initial and boundary conditions.

Future releases of TUFLOW FV will allow alternative methods for specification of initial and boundary conditions that do not rely on assumed ordering. In the interim however, the following applies.

4.4.2.3.1 Initial Conditions

Initial conditions, if set using means other than a restart file, must be specified with water quality constituents in a preset order (globally uniform), or be referenced using incrementally numbered headers as “wq_1”, “wq_2” etc (profile, 2D or 3D, see Section 4.4.2.1).

For globally uniform initial conditions (Section 4.4.2.1.2), the following *.fvc command can be used for a typical inorganics simulation class:

```
Initial WQ Concentration == 7.5, 0.0, 4.2, 10.5, 0.6, 5.5
```

There are no references to headers or variable names, but TUFLOW FV assumes that these numbers correspond to the ordered variables of the particular configuration of the inorganics simulation class returned to it from the WQ Module. In this example, this ordering is:

- Dissolved oxygen (7.5 mg/L)
- Silicate (0.0 mg/L)
- Ammonium (4.2 mg/L)
- Nitrate (10.5 mg/L)
- Filterable reactive phosphorus (0.6 mg/L), and
- One phytoplankton group (5.5 $\mu\text{g/L}$)

The expected ordering is the same as that for boundary condition specifications, as described below.

For other initial condition specifications that involve providing csv files, the headers “wq_1”, “wq_2” etc must be used to denote water quality initial conditions. The ordering of the associated columns does not matter, however the assignment of a computed variable initial condition to a “wq_xx” header (where xx is a number) does rely on the ordering described below - the first water quality computed variable expected should be headed “wq_1” and so on.

4.4.2.3.2 Boundary Conditions

Ordering of water quality boundary conditions is only important when specifying header information via the **BC Header ==** (or equivalent) command within a TUFLOW FV *.fvc file BC block. It is in these commands (where comma separated header strings are specified) that TUFLOW FV expects a particular order of TUFLOW FV and WQ Module constituents. No column ordering is expected in boundary condition data files themselves. Ordering is only expected in the order of headers specified within a BC block within an TUFLOW FV control file. This is best illustrated by example.

If a user has elected to deploy the inorganics simulation class without sediment, then the following will be simulated (beyond the basic velocity and water level hydrodynamic variable suite):

- Salinity
- Temperature
- Dissolved oxygen
- Silicate
- Ammonium
- Nitrate
- Filterable reactive phosphorus
- One (assumed for this example, but can be multiple) phytoplankton group

These will eventually need proper boundary condition specification in boundary condition blocks and have supporting data provided in (usually) text files. In a simple model with only one WL boundary condition, a BC block of the following form would be required as a minimum to properly specify the hydrodynamic and water quality boundaries:

```
BC == WL, 1, datafile.csv
  BC Header == Time, WSE1, Sali, Temp, DOxy, SiO4, NH41, Nitr, FRPh, Bluegreen
End BC
```

To be clear:

- The names listed on the “**BC Header ==**” line (time, wse etc.) are not keywords or special names, and can be any names that a user chooses
- TUFLOW FV will however, assume that these names (whatever they have been set to) have been listed in such an order that they have a one to one correspondence to the ten computed variables as follows:
 1. Time → Time stamp
 2. WSE1 → Water surface elevation
 3. Sali → Salinity
 4. Temp → Temperature
 5. DOxy → Dissolved oxygen
 6. SiO4 → Silicate
 7. NH41 → Ammonium

8. `Nitr` → Nitrate
 9. `FRPh` → Filterable reactive phosphorus
 10. `Bluegreen` → Phytoplankton group one
- TUFLOW then matches the user specified names to the expected simulation variables, based on this ordering, to then interrogate boundary condition files.

Following the above matching, TUFLOW FV interrogates the relevant boundary condition file (“`datafile.csv`” in the example above), where this file can have its columns arranged in any order: the order of these columns does not matter because TUFLOW FV will use the mapping previously developed via the `BC Header ==` command to look through all data file columns one by one, searching for the headers specified, regardless of the actual ordering of boundary condition file columns. For example, the silicate boundary condition data could be positioned in column 14 of the boundary condition file, but as long as it is labelled with the correct header (“`SiO4`” as specified in `BC Header ==`), TUFLOW FV will know to assign column 14 of the boundary condition data file to the silicate computed variable.

Ordering is set by the user’s selection of simulation class and constituent models, and is explicitly listed in each simulation class section (Section 4.6.5, Section 4.7.5 and Section 4.8.5 for DO, inorganics and organics, respectively). The expected ordering for a particular simulation is also reported in the simulation water quality log file for checking.

4.5 Water quality control file commands

The water quality control file comprises three parts, with each part containing different types of commands and flags. Whilst it is recommended that these parts be kept separate and in the order described below (especially given how complex water quality simulations can become), doing so is not mandatory and commands or command blocks may be entered in any order.

These parts are as follows, with the first two mirroring the architecture described in Chapter 2:

1. Simulation controls (i.e. simulation class)
2. Constituent model settings (i.e. constituent model class)
3. Material specifications

Notwithstanding this, a WQ Module control file need not contain any commands, and can be completely blank. This is by design, and intended to allow users to rapidly set up and execute a TUFLOW water quality simulation. If the water quality control file is left blank, then the WQ Module will:

- Construct a simulation using the dissolved oxygen simulation class (which is the simplest class)
- Set the simulation units to mg/L
- Set library defaults for all parameters
- Set the water quality model timestep to the default
- Assign zero dissolved oxygen concentration to all boundary conditions. This is by design, and will assist in ensuring that the subsequent user-defined updating of boundary conditions is thorough and complete (zero dissolved oxygen boundary conditions are rare and therefore easily identifiable).

Initial conditions will also need to be specified in the TUFLOW FV control file as per Section 4.4.2. Specification of boundary conditions can be deferred.

The water quality control file sections are described below. Details specific to each simulation class and constituent model are provided in subsequent sections

4.5.1 Part 1: Simulation controls

Simulation controls set the high level operation of the WQ Module and are not specific to a simulation class. All are optional. Available commands set the:

- Simulation class via `simulation class ==`
- Timestep `dt` (in seconds) at which TUFLOW calls the WQ Module via `wq dt ==`
- Units of simulation via `wq units ==`
- Frequency of equilibrium substepping `Fess` (in number of timesteps) to execute non-kinetic equilibrium calculations via `wq Equilibrium Substeps ==`
- Reporting or suppression of minimum / maximum concentration exceedances (see Section 4.5.2) via `Report Min Max warnings ==`

A typical simulation control section might therefore look like the following:

```
Simulation Class == DO
WQ dt == 600.0
WQ Units == Mg/L
WQ Equilibrium Substeps == 1
Report Min Max Warnings == ON
```

4.5.2 Part 2: Constituent model settings

Constituent model settings are those that:

- Specify the constituent model to be used within each preset constituent model class. These are referred to as constituent model blocks
- Set the parameters for each of these constituent models, as commands within these blocks

All are optional, however if a constituent model block is initiated then it requires an `End xxxx Model` command to terminate the block, where `xxxx` is the name of the constituent model class, such as inorganic nitrogen. An example of a user selecting to use the adsorbed filterable reactive phosphorous constituent model (that is a model available within the inorganic phosphorus constituent model class), and setting some parameters within that model is as follows:

```
Inorganic Phosphorus Model == FRPads
    Atmospheric Deposition == 12.6, 0.5
End Inorganic Phosphorus Model
```

Parameters not specified by the user are set to library defaults.

All constituent models allow for constraining (and then reporting) the predictions of their respective computed variable concentrations via the setting of minimum and maximum limits, if desired. This is often useful in identifying unusual model behaviours or instabilities. Where exceedences of these limits are identified by the WQ Module:

- Time and model cell information is written to the WQ Module log file in real time. This allows for easy identification of potential model issues via periodic examination of the WQ Module log file, rather than waiting for simulation completion
- The WQ Module resets the computed concentration to the relevant specified minimum or maximum concentration

The above resetting will result in mass conservation errors. It should not be relied on to artificially control the behaviour of an otherwise unstable or runaway water quality simulation. Rather, this functionality should be used as a convenient way to check model performance and flag potential issues, with a view to then implementing corrective action. Equally, suppressing warnings written to the WQ log file using the `Report Min Max Warnings ==` command described in Section 4.5.1 is not recommended because doing so may mask underlying model construction issues.

These limits are optionally specified in each constituent model block. An example that sets these limits for ammonium is:

```
Ammonium Min Max == 0.0, 25.0
```

Although in the strictest sense, sediment (benthic) flux half saturation concentrations and temperature coefficients are benthic properties, the WQ Module does not yet support these parameters being applied on a spatially varying basis (i.e. per material). As such, these are considered to be constituent model global parameters and so are set in this part of the water quality control file, i.e. within respective constituent model blocks. An example that sets an oxygen half saturation and temperature coefficient for benthic flux is:

```
Oxygen Benthic == 5.0, 1.08
```

4.5.3 Part 3: Material specifications

The final part of the water quality control file (*.fwq) provides for specification of benthic (sediment) fluxes, via material blocks. The commands required to commence and terminate a materials block are as follows:

```
Material == <_up to 10 comma separated material numbers, or ``default''_>
```

and

```
End Material
```

This material block nomenclature mirrors that used in the TUFLOW FV and sediment transport control files. An example of specifying oxygen and nitrate benthic fluxes for materials 2, 7 and 12 is:

```
Material == 2, 7, 12
    Oxygen Flux == -60.0
    Nitrate Flux == 12.5
End Material
```

The WQ Module allows for specification of a default set of benthic fluxes that are applied across all materials, by using the key word `Default` instead of specifying material numbers in a material block. These defaults can then be progressively overwritten on a material by material basis by specifying subsequent material blocks.

For example, a model that has ten materials in total, eight of which have the same oxygen benthic flux (all materials except 4 and 7), can have its overall oxygen benthic flux specified as:

```
Material == Default
    Oxygen Flux == -60.0
End Material

Material == 4, 7
    Oxygen Flux == -20.0
End Material
```

4.5.4 Summary

In order to set up and execute a water quality simulation using the WQ Module, the following steps are required:

- Modify the TUFLOW FV control file:
 - Add at least the following commands to TUFLOW FV control file (*.fvc):
 - * `Water Quality Model == TUFLOW`
 - * `Water Quality Control File == <water quality control file name>.fvwq`
 - Optionally add a folder path command to the TUFLOW FV control file (*.fvc) with a trailing backslash:
 - * `Water Quality Model Dir == <relative path to *.fvwq file>\`
 - Add appropriate initial conditions for all water quality constituents, observing ordering rules where required
 - Initially optionally add boundary conditions for all water quality constituents, observing ordering rules in `BC Header == commands`
- Create the water quality control file with the corresponding name and path
- Modify the water quality control file
 - Optionally add to the water quality control file:
 - * Part 1: A simulation controls section
 - * Part 2: A constituent model setting section with one or more constituent model blocks with one or more parameter commands
 - * Part 3: A material block specifications section

Once initially constructed, boundary conditions can be added (if not already in place), and progressive refinement and parameterisation of constituent models and benthic fluxes can be affected. Details of these commands and their options within each specific simulation class are provided in subsequent sections. Subsections are separated into the above water quality control file parts for ease and consistency of reference. All commands are optional.

4.5.5 Log files

Every WQ Module water quality simulation generates a log file that contains an echo of the WQ Module construction and execution commentary. It is written to the same location (and with the same name) as the WQ Module control file, with the file extension “fvwqlog”. This file contains a great deal of information that should be carefully reviewed. Suppressing warnings written to this log file, although possible, is not recommended or encouraged.

4.6 Simulation Class: DO

If no simulation class is specified then a simulation will be automatically constructed using this DO class, and populated with library defaults for all parameters. Computed variables will be:

- Dissolved oxygen
- Pathogens (optional, potentially multiple)

4.6.1 Prerequisites

The DO simulation class requires simulation of the following in TUFLOW FV:

- Hydrodynamics, in either two or three dimensions (including any internal one dimensional structures if present)
- Salinity
- Temperature
- Heat module on (i.e. meteorological forcing is required)

Simulation of suspended sediment (via TUFLOW FV's sediment transport module) is optional, unless attached pathogens are simulated.

4.6.2 Part 1: Simulation specification

The DO simulation class is set via

```
Simulation Class == DO
```

The other commands in this part are not specific to this simulation class. See Section 4.5.1.

4.6.3 Part 2: Constituent model specification

As per Table 2.2 and Table 2.3, oxygen is the only mandatory constituent model class available within the DO simulation class, and there is only one oxygen constituent model within that class, with code O2. Pathogens may be optionally simulated (in any simulation class).

4.6.3.1 Model class: Oxygen

4.6.3.1.1 Constituent model: O2

This constituent model is specified as:

```
Oxygen Model == O2
```

Minimum and maximum concentrations are specified as:

```
oxygen Min Max ==  $[DO]_{min}^{O_2}, [DO]_{max}^{O_2}$ 
```

Global benthic parameters (used in Equation C.6) are specified as:

```
Oxygen Benthic ==  $K_{sed-O_2}^{O_2}, \theta_{sed}^{O_2}$ 
```

The oxygen piston model to be used (in either Equation C.2 or Equation C.3) is specified as:

```
Oxygen Piston Model == Wanninkhof92
```

or

```
Oxygen Piston Model == Ho16
```

The argument (either “Wanninkhof92” or “Ho16”) activates a different oxygen piston model (Equation C.2 or Equation C.3, respectively).

Although not strictly necessary, the use of “oxygen” to prefix these block commands is deliberate so as to maintain consistency of command style with other constituent model blocks that include more than one computed variable, such as nitrogen, phosphorus and organics. Nonetheless, if the “oxygen” prefix is omitted within this constituent model block, the WQ Module will still interpret the above commands correctly.

This constituent model block must be terminated using the command:

```
End Oxygen Model
```


4.6.3.2 Model class: Pathogens (optional)

This model class is optional.

4.6.3.2.1 Constituent model: Free

This constituent model is specified as:

Pathogen Model == Free, <pathname>

<pathname> is any user specified pathogen group name that:

- Uses only alphanumeric characters
- Has no spaces
- Excludes the keyword 'PATH', and
- Is not the same as any other group name

Minimum and maximum concentrations are specified as:

Alive Min Max == $[PTH_a]_{min}^{pth}$, $[PTH_a]_{max}^{pth}$

Mortality parameters are specified as:

Mortality == k_d^{pth} , C_{SM}^{pth} , α , β , θ_{mor}^{pth}

$[\beta]$ is not currently used but must be retained as a placeholder in this command for future use.

Light inactivation parameters are specified in three separate but related commands, with one command per light band (visible, UV-A and UV-B):

Visible Inactivation == k_{vis}^{pth} , $c_{S_{vis}}^{pth}$, $K_{DO_{vis}}^{pth}$

UVA Inactivation == k_{uva}^{pth} , $c_{S_{uva}}^{pth}$, $K_{DO_{uva}}^{pth}$

UVB Inactivation == k_{uvb}^{pth} , $c_{S_{uvb}}^{pth}$, $K_{DO_{uvb}}^{pth}$

Settling of non-attached pathogens is specified as follows, with a negative number being a downwards velocity:

Settling == V_{settle}^{pth}

This constituent model block must be terminated using the command:

End Pathogen Model

4.6.3.2.2 Constituent model: Attached

This constituent model must be accompanied by simulation of at least one sediment fraction within the TUFLOW FV sediment transport (ST) module, and is specified as:

Pathogen Model == Attached, <pathname>

<pathname> is any user specified pathogen group name that:

- Uses only alphanumeric characters
- Has no spaces
- Excludes the keyword 'PATH', and
- Is not the same as any other group name

The commands are the same as those specified within a free pathogen constituent model block (Section 4.6.3.2.1), with the following modification or additions.

Settling is specified for both free and attached pathogens:

Settling == V_{settle}^{pth} , $V_{settle}^{pth_t}$

The target attached pathogen fraction is specified as:

Target Attached Fraction == f_{att}^{pth}

This constituent model block must be terminated using the command:

End Pathogen Model

4.6.4 Part 3: Material specification

Oxygen benthic flux (used in Equation C.6) is specified within both default and numbered material blocks as:

Oxygen Flux == $F_{sed}^{O_2}$

4.6.5 Constituent ordering

Dissolved oxygen is the only mandatory constituent simulated by the WQ Module for this simulation class, and therefore oxygen concentration is specified as the first variable (shown in symbolic form below):

Initial WQ Concentration == [DO]

Similarly, in a BC Header == command within a BC block, oxygen is expected to be the first and only mandatory water quality variable after hydrodynamic boundary conditions.

BC Header == Time, water_Elev, Sal, Temp, Clay, Sand, DO_mgL

DO_mgL is the header used to designate oxygen in the related boundary condition file, noting that the DO_mgL column in the boundary condition file can appear in any column in the boundary condition file, and that it does not need to be the seventh column. The header text “DO_mgL” is just an example, and it can be any header desired, as long as it matches the correct column header in the boundary condition file.

4.6.5.1 Pathogens (optional)

If pathogens are simulated, then their headers are required at the end of any lists, regardless of the other hydrodynamic and water quality constituents simulated. This therefore applies to all simulation classes from DO to organics. Alive and dead pathogens are always required to be specified, in that order, and if attached pathogens are simulated then that attached pathogens header is listed between those of alive and dead. This pattern is repeated for each specified pathogen group, in the order in which pathogen groups are defined via pathogen constituent model blocks in the water quality control file. For example, where two pathogen groups are simulated (called ECOLI and CRYPTO, and defined in that order in the corresponding water quality control file), with ECOLI including attachment, the above BC header would be extended to the following:

BC Header == Time, water_Elev, Sal, Temp, Clay, Sand, DO_mgL, ECOLI_alive, ECOLI_att,
↪ ECOLI_dead, CRYPTO_al, CRYPTO_de

4.6.6 Example

Following is an example of all the available WQ Module Simulation Class == DO commands. A single material applied as zeros everywhere as the default, other than for materials 1 and 4 where the default flux is overwritten. One (optional) pathogen constituent model block has been included, but is not required.

Example - Simulation Class == DO

```
Simulation Class == DO
WQ dt == 600
WQ Units == MgL

Oxygen Model == O2
  Oxygen Benthic == 4.0, 1.05
  Oxygen Min Max == 0.0, 15.0
End Oxygen Model

! Optional Pathogen Constituent Model Block
Pathogen Model == Free, Crypto
  Alive Min Max == 0.0, 1e7
  Mortality == 0.08, 2e-12, 6.1, 1.0, 1.11
  Visible Inactivation == 0.082, 0.0067, 0.5
```

```

    UVA Inactivation == 0.5, 0.0067, 0.5
    UVB Inactivation == 1.0, 0.0067, 0.5
    Settling == -0.03
End Pathogen Model

Material == Default
    Oxygen Flux == 0
End Material

Material == 1, 4
    Oxygen Flux == -137.0
End Material

```

4.7 Simulation Class: Inorganics

If the inorganics simulation class is specified with no subsequent constituent model blocks, then a simulation will be automatically constructed using this inorganics class, and populated with library defaults for all parameters. Computed variables will be:

- Dissolved oxygen
- Silicate
- Ammonium
- Nitrate
- Filterable reactive phosphorus
- One phytoplankton group named 'dummy' that uses the basic phytoplankton constituent model

4.7.1 Prerequisites

The inorganics simulation class requires simulation of the following in TUFLOW FV:

- Hydrodynamics, in either two or three dimensions (including any internal one dimensional structures if present)
- Salinity
- Temperature
- Heat module on (i.e. meteorological forcing is required)

Simulation of suspended sediment (via TUFLOW FV's sediment transport module) is required only if adsorbed phosphorus is to be simulated by the WQ Module. This is affected through specification of the adsorbed phosphorus constituent model within the phosphorus constituent model class.

4.7.2 Part 1: Simulation specification

The inorganics simulation class is set via

```
Simulation Class == Inorganics
```

The other commands in this part are not specific to this simulation class. See Section 4.5.1.

4.7.3 Part 2: Constituent model specification

As per Table 2.2 and Table 2.3, there are several constituent model classes available within the inorganics simulation class. The commands for each are described following.

4.7.3.1 Model class: Oxygen

4.7.3.1.1 Constituent model: O2

The commands for this constituent model are described in Section 4.6.3.1.1.

4.7.3.2 Model class: Silicate

4.7.3.2.1 Constituent model: Si

This constituent model is specified as:

```
Silicate Model == Si
```

Minimum and maximum concentrations are specified as:

```
Silicate Min Max == [Si]minSi, [Si]maxSi
```

Global benthic flux parameters (used in Equation D.1) are specified as:

```
Silicate Benthic == Ksed-O2Si, θsedSi
```

Although not strictly necessary, the use of “silicate” to prefix the above block commands is deliberate so as to maintain consistency of command style with other constituent model blocks that include more than one computed variable, such as nitrogen, phosphorus and organics.

Silicate sediment flux calculations are set to be dependent on dissolved oxygen concentrations by default. Although not recommended, the following will switch off this dependence by setting the term labelled “Influence of oxygen” in Equation D.1 to a value of 1.0.

```
Oxygen == OFF
```

This constituent model block must be terminated using the command:

```
End Silicate Model
```

4.7.3.3 Model class: Inorganic nitrogen

4.7.3.3.1 Constituent model: AmmoniumNitrate

This constituent model is specified as:

```
Inorganic Nitrogen Model == AmmoniumNitrate
```

Minimum and maximum concentrations for both ammonium and nitrate are specified as:

```
Ammonium Min Max == [NH4]minNH4, [NH4]maxNH4
```

```
Nitrate Min Max == [NO3]minNO3, [NO3]maxNO3
```

Global benthic flux parameters (used in Equation E.1) for ammonium and nitrate are specified as:

```
Ammonium Benthic == Ksed-O2NH4, θsedNH4
```

```
Nitrate Benthic == Ksed-O2NO3, θsedNO3
```

Nitrification parameters (used in Equation E.3 and therefore Equation E.4) are set in a single command as:

```
Nitrification == RnitrifNH4, Knitrif-O2NH4, θnitrifNH4
```

Denitrification parameters (used in Equation E.5 or Equation E.6) are also set in a single command as:

```
Denitrification == Michaelis Menten, RdenitNO3, Kdenit-O2-MMNO3, θdenitNO3
```

or

```
Denitrification == Exponential, RdenitNO3, Kdenit-O2-expNO3, θdenitNO3
```

The first argument (either “Michaelis Menten” or “Exponential”) activates a different denitrification model (Equation E.5 or Equation E.6, respectively).

Anaerobic oxidation of ammonium parameters (used in Equation E.10) are also set in a single command as:

```
Anaerobic Oxidation Of Ammonium == RanmxNH4,NO3, Kanmx-NH4NH4,NO3, Kanmx-NO3NH4,NO3
```

Dissimilatory reduction of nitrate to ammonium parameters (used in Equation E.11) are set in a single command as:

Diss Nitrate Reduction To Ammonium == $R_{DRNA}^{NO_3}, K_{DRNA-O_2}^{NO_3}$

Ammonium and nitrate sediment flux, nitrification, denitrification, anammox and DRNA calculations are all set to be dependent on dissolved oxygen concentrations by default. Although not recommended, the following will switch off this dependence for all these processes.

Oxygen == OFF

This command overrides any previously specified values of $K_{sed-O_2}^{NH_4}$, $K_{sed-O_2}^{NO_3}$, $K_{nitrif-O_2}^{NH_4}$, $K_{denit-O_2-MM}^{NO_3}$ and $K_{denit-O_2-exp}^{NO_3}$. It should be specified after all other related commands if the influence of oxygen on nitrogen processes is to be switched off. Setting this command to 'OFF' will completely disable anammox and DRNA calculations.

Atmospheric deposition parameters (used in Equation E.13, Equation E.14, Equation E.17 and Equation E.18) are set via the command:

Atmospheric Deposition == $[TN]_{rain}, R_{atm-dry}^{TN}, f_{TN}^{NO_3}$

The same split of TN into ammonium and nitrate is applied to both $[TN]_{rain}$ and $R_{atm-dry}^{TN}$.

This constituent model block must be terminated using the command:

End Inorganic Nitrogen Model

4.7.3.4 Model class: Inorganic phosphorus

4.7.3.4.1 Constituent model: FRPhs

This constituent model is specified as:

Inorganic Phosphorus Model == FRPhs

Minimum and maximum concentrations for FRP are specified as:

FRP Min Max == $[FRP]_{min}^{FRP}, [FRP]_{max}^{FRP}$

Global benthic flux parameters (used in Equation F.1) are specified as:

FRP benthic == $K_{sed-O_2}^{FRP}, \theta_{sed}^{FRP}$

FRP sediment flux calculations are set to be dependent on dissolved oxygen concentrations by default. Although not recommended, the following will switch off this dependence by setting the term labelled "Influence of oxygen" in Equation F.1 to a value of 1.0.

Oxygen == OFF

Wet atmospheric deposition parameters (used in Equation F.2) are set via the command:

Atmospheric Deposition == $[FRP]_{rain}$

An additional parameter for dry atmospheric deposition is required in the FRPhsAds constituent model (see Section 4.7.3.4.2).

This constituent model block must be terminated using the command:

End Inorganic Phosphorus Model

4.7.3.4.2 Constituent model: FRPhsads

This constituent model is specified as:

Inorganic Phosphorus Model == FRPhsAds

The TUFLOW FV Sediment Transport (ST) Module must be used to simulate at least one sediment fraction in order to use this WQ Module constituent model.

In addition to the commands described in Section 4.7.3.4.1, the following commands are available in this constituent model.

Minimum and maximum concentrations for adsorbed FRP are specified as:

$FRP\ Ads\ Min\ Max == [FRPads]_{min}^{FRPads}, [FRPads]_{max}^{FRPads}$

Two FRP adsorption models are available, as per Equation F.6 and Equation F.7. These require specification of one (linear) or two (quadratic) parameters, respectively after specification of the model to be used:

$Adsorption == Linear, K_{ads-L}^{FRP}$

or

$Adsorption == Quadratic, K_{ads-Q}^{FRP}, Q_{max}^{FRP}$

The settling velocity of adsorbed phosphorus is set as follows. Future releases of the WQ Module will dynamically link this settling velocity to the calculations of the TUFLOW FV ST Module.

$Settling == V_{settle}^{FRPads}$

Dry atmospheric deposition of FRP is activated in this simulation model (used in Equation F.3) and is specified via the same command as wet deposition, but with one additional argument. This additional argument is ignored if the FRPhsAds constituent model has not been set:

$Atmospheric\ Deposition == [FRP]_{rain}, R_{atm-dry}^{FRP}$

This constituent model block must be terminated using the command:

End Inorganic Phosphorus Model

4.7.3.5 Model class: Phytoplankton

Given the large number of potential commands and options for phytoplankton simulation, horizontal rules have been used to separate subsections below for clarity.

4.7.3.5.1 Constituent model: Basic

This constituent model is specified as:

Phyto Model == Basic, groupname

‘groupname’ is any user specified phytoplankton group name that:

- Uses only alphanumeric characters
- Has no spaces
- Excludes the keywords ‘COM’ and ‘PHYTO’, or any combination of letters already included in a standard computed variable name, such as “INT_N_”, “INT_P” or “_rho”, and
- Is not the same as any other group name

Minimum and maximum concentrations for a phytoplankton group are specified as follows. No prefix keyword (as was the case for constituents such as “ammonium”) is required:

$Min\ Max == [PHY]_{min}^{PHY}, [PHY]_{max}^{PHY}$

4.7.3.5.1.1 Temperature limitation

Temperature limitation can be specified by one of the following models:

- None (no temperature limitation applied)

Temperature Limitation == None

or

- Standard (used in Equation I.1 through to Equation I.8)

Temperature limitation == Standard, T_{std}^{phy} , T_{opt}^{phy} , T_{max}^{phy}

4.7.3.5.1.2 Salinity limitation

Salinity limitation can be specified by one of the following models. All functions can be applied to either (not both) primary productivity or respiration, except for the estuarine limitation model which can only be applied to primary productivity. Specifically:

- Specifying respective function limitation values (i.e. $L_{max-fresh}^{phy}$ or $L_{zero-marine}^{phy}$ or $L_{zero-mix}^{phy}$) to be between zero and one will set a function to apply to primary productivity rates as a reducer
- Specifying respective function limitation values (i.e. $L_{max-fresh}^{phy}$ or $L_{zero-marine}^{phy}$ or $L_{zero-mix}^{phy}$) to be greater than one will set a function to apply to respiration rates as an enhancer

The available models are as follows:

- None (no salinity limitation applied)

`Salinity Limitation == None`

or

- Fresh (used in Equation I.27)

`Salinity Limitation == Fresh,  $S_{opt-fresh}^{phy}$ ,  $S_{max-fresh}^{phy}$ ,  $L_{max-fresh}^{phy}$`

or

- Marine (used in Equation I.30)

`Salinity Limitation == Marine,  $S_{opt-marine}^{phy}$ ,  $L_{zero-marine}^{phy}$`

or

- Mixed (used in Equation I.33)

`Salinity Limitation == Mixed,  $S_{opt-mix}^{phy}$ ,  $S_{max-mix}^{phy}$ ,  $L_{zero-mix}^{phy}$`

or

- Estuarine (used in Equation I.36)

`Salinity Limitation == Estuarine,  $S_{opt-est}^{phy}$ ,  $S_{max-est}^{phy}$ ,  $P_{est}^{phy}$`

4.7.3.5.1.3 Light limitation

Light limitation can be specified by one of the following models:

- Basic (used in Equation I.19)

`Light Limitation == Basic,  $Ke^{phy}$ ,  $I_{K-bas}$`

or

- Monod (used in Equation I.20)

`Light Limitation == Monod,  $Ke^{phy}$ ,  $I_{K-mon}$`

or

- Steele (used in Equation I.21)

`Light Limitation == Steele,  $Ke^{phy}$ ,  $I_{S-ste}$`

or

- Webb (used in Equation I.22)

`Light Limitation == webb,  $Ke^{phy}$ ,  $I_{K-webb}$`

or

- Jassby (used in Equation I.23)

`Light Limitation == Jassby,  $Ke^{phy}$ ,  $I_{K-jas}$`

or

- Chalker (used in Equation I.24)

`Light Limitation == Chalker,  $K_e^{phy}$ ,  $I_{K-cha}$`

or

- Klepper (used in Equation I.25)

`Light Limitation == Klepper,  $K_e^{phy}$ ,  $I_{S-kle}$`

or

- Integrated (used in Equation I.26)

`Light Limitation == Integrated,  $K_e^{phy}$ ,  $I_{S-int}$`

4.7.3.5.1.4 Nitrogen limitation

Nitrogen limitation parameters (used in Equation I.9, Section I.3.1) are set via the command:

`Nitrogen Limitation ==  $[N]_{min}^{phy}$ ,  $K_{lim-N}^{phy}$`

These, together with additional parameters, are the same as those used in specifying the nitrogen limitation behaviour of the advanced phytoplankton model (Section 4.7.3.5.2.1).

4.7.3.5.1.5 Phosphorus limitation

Phosphorus limitation parameters (used in Equation I.13, Section I.4.1) are set via the command:

`Phosphorus Limitation ==  $[P]_{min}^{phy}$ ,  $K_{lim-P}^{phy}$`

These, together with additional parameters, are the same as those used in specifying the phosphorus limitation behaviour of the advanced phytoplankton model (Section 4.7.3.5.2.2).

4.7.3.5.1.6 Silicate limitation

Silicate limitation parameters (used in Equation I.17, Section I.5) are set via the command:

`silicate Limitation ==  $[Si]_{min}^{phy}$ ,  $K_{lim-Si}^{phy}$`

Specification of this limitation triggers the uptake of silicate to be on in the phytoplankton group's block in which the command appears. Omit this command to set silicate uptake to off for a given phytoplankton group.

4.7.3.5.1.7 Uptake

Nutrient uptake parameters for nitrogen, phosphorus and silicate (if relevant) (used in Equation J.2, Equation J.7 and Equation J.9 respectively) are set via the command:

`uptake ==  $X_{N-C-con}^{phy}$ ,  $X_{P-C-con}^{phy}$ ,  $X_{Si-C-con}^{phy}$`

If specified, the value of $X_{Si-C-con}^{phy}$ is ignored if silicate uptake has not been triggered via specification of silicate limitation parameters via `Silicate Limitation ==`.

4.7.3.5.1.8 Primary productivity

Primary productivity (growth) parameters (used in Equation H.2) are set via the command:

`Primary Productivity ==  $R_{prod}^{phy}$ ,  $\theta_{prod}^{phy}$`

4.7.3.5.1.9 Respiration

Respiration parameters are set via the following command. The first two parameters are used directly to compute the respiration rate $R_{resp(computed)}^{phy}$ via Equation H.6. The third and fourth parameters are used to compute excretive and mortality fluxes in Equation K.1 and Equation K.2, respectively. Both these equations use the respiration rate computed from the first two parameters R_{resp}^{phy} and θ_{resp}^{phy} . Although not strictly related to respiration, the final parameter does represent a reduction of biomass and is used to compute exudation loss using Equation H.12.

`Respiration ==  $R_{resp}^{phy}$ ,  $\theta_{resp}^{phy}$ ,  $f_{true-resp}^{phy}$ ,  $f_{excr-loss}^{phy}$ ,  $f_{exud}^{phy}$`

4.7.3.5.1.10 Carbon to Chlorophyll *a* ratio

The carbon to chlorophyll *a* ratio (used in converting between simulation units, and reporting total chlorophyll *a* as a diagnostic variable if the mmol units system is used) is specified via the command:

`Carbon Chla Ratio ==  $X_{cc}^{phy}$`

4.7.3.5.1.11 Nitrogen fixing

Nitrogen fixing parameters are specified as follows. The first parameter is used in Equation J.2 to compute the nitrogen fixation flux, and the second parameter modifies computed primary productivity via Equation H.3.

`Nitrogen Fixing ==  $R_{nfix}^{N_2}, f_{nfix}^{phy}$`

Setting this command triggers nitrogen fixing to be on, otherwise it is off by default.

4.7.3.5.1.12 Settling

Settling can be specified by one of the following models:

- None

`Settling == None`

or

- Constant

`Settling == Constant,  $V_{settle}^{phy}$`

or

- Constant with density correction (as per Equation H.18)

`Settling == Thermal,  $V_{settle}^{phy}$`

or

- Stokes (used in Equation H.19), where density is required to be simulated as a computed variable, and thus requires the specification of I_K .

`Settling == Stokes,  $I_{K-sto}$`

If I_K is specified in any light limitation model applied to a phytoplankton group with stokes settling, then a value of I_{K-sto} specified in the stokes model will be ignored. Cell density limits are applied as the defaults and are not user specifiable.

4.7.3.5.1.13 Termination

This constituent model block must be terminated using the command:

`End Phyto Model`

4.7.3.5.2 Constituent model: Advanced

This constituent model is specified as:

`Phyto Model == Advanced, groupname`

'groupname' is any user specified phytoplankton group name that:

- Uses only alphanumeric characters
- Has no spaces
- Excludes the keywords 'COM' and 'PHYTO', or any combination of letters already included in a standard computed variable name, such as "INT_N_", "INT_P" or "_rho", and
- Is not the same as any other group name

The following commands are the same as those described for the basic phytoplankton model in Section 4.7.3.5.1 (links are to relevant sections above rather than to the command Appendix, for ease of cross reference):

Min Max ==

Temperature Limitation ==

Light Limitation ==

Silicate Limitation ==

Primary Productivity ==

Respiration ==

Carbon Chla Ratio ==

Nitrogen Fixing ==

Settling ==

End Phyto Model ==

The following commands differ for the advanced phytoplankton model compared to the basic model.

4.7.3.5.2.1 Nitrogen limitation

Nitrogen limitation parameters (used in Equation I.11, Section I.3.2) are set via the command:

Nitrogen Limitation == $[N]_{min}^{phy}, K_N^{phy}, X_{N-C-min}^{phy}, X_{N-C-max}^{phy}$

The first two parameters are the same as those that would be specified using the same command in the basic phytoplankton model (Section 4.7.3.5.1.4).

4.7.3.5.2.2 Phosphorus limitation

Phosphorus limitation parameters (used in Equation I.15, Section I.4.2) are set via the command:

Phosphorus Limitation == $[P]_{min}^{phy}, K_P^{phy}, X_{P-C-min}^{phy}, X_{P-C-max}^{phy}$

The first two parameters are the same as those that would be specified using the same command in the basic phytoplankton model (Section 4.7.3.5.1.5).

4.7.3.5.2.3 Uptake

Nutrient uptake parameters for nitrogen, phosphorus and silicate (if relevant) (used in Equation J.4, Equation J.8 and Equation J.9 respectively) are set via the command:

Uptake == $R_{N-uptake}^{phy}, R_{P-uptake}^{phy}, X_{Si-C-con}^{phy}$

The value of $X_{Si-C-con}^{phy}$ is ignored if silicate uptake has not been triggered through specification of a silicate limitation function.

4.7.3.5.2.4 Settling

An additional settling model can be specified in the advanced phytoplankton constituent model as:

- Motile (Section H.4.5), where internal nutrient simulation is required to simulate motility

Settling == Motile, V_{mot}^{phy}, I_{K-mot}

If I_K is specified in any light limitation model applied to an advanced constituent model phytoplankton group with motile settling, then a value of I_{K-mot} specified in the motile model will be ignored. Cell density limits are applied as the defaults and are not user specifiable.

This constituent model block must be terminated using the command:

End Phyto Model

4.7.3.6 Model class: Pathogens (optional)

This model class is optional.

4.7.3.6.1 Constituent model: Free

The commands for this constituent model are described in Section 4.6.3.2.1.

4.7.3.6.2 Constituent model: Attached

The commands for this constituent model are described in Section 4.6.3.2.2.

4.7.4 Part 3: Material specification

Oxygen, silicate, ammonium, nitrate and FRP benthic fluxes are specified within both default and numbered material blocks as:

```
Oxygen Flux ==  $F_{sed}^{O_2}$ 
Silicate Flux ==  $F_{sed}^{sil}$ 
Ammonium Flux ==  $F_{sed}^{NH_4}$ 
Nitrate Flux ==  $F_{sed}^{NO_3}$ 
FRP Flux ==  $F_{sed}^{FRP}$ 
```

No adsorbed FRP or phytoplankton sediment fluxes are required.

4.7.5 Constituent ordering

Different constituent model selections result in different ordering requirements for specifying computed variable initial conditions (either globally with an implied order, or setting the ordered map from water quality computed variables to “wq_1”, “wq_2” etc) and **BC Header ==** commands. For clarity, these are initially presented below using only phytoplankton placeholders in lists. This is possible because phytoplankton specifications are always appended at the end of initial condition or “**BC Header ==**” lists. Phytoplankton specifications are then presented as additive to these lists in subsequent sections. This is not meant to imply that phytoplankton simulation is optional in the inorganics simulation class - it is mandatory and has only been described separately here only for clarity of presentation.

4.7.5.1 Excluding phytoplankton

The only constituent model choice that influences ordering (other than phytoplankton) is the phosphorus model. These two possibilities are described below.

4.7.5.1.1 Phosphorus model FRPhs

If adsorbed FRP is not simulated (i.e. **Phosphorus Model == FRPhs**), then in all columnar and list style initial conditions, computed variables are expected in the following order (and map to “wq_1” etc accordingly):

```
Initial WQ Concentration == [DO], [Si], [NH4], [NO3], [FRP], ... {phytoplankton placeholder/s}
```

Similarly, in a **BC Header ==** command within a BC block, the following order of computed variables is expected after hydrodynamic (HD BCs) boundary conditions:

```
BC Header == {HD BCs} ... DO_mgL, Si_mgL, Amm_mgL, Nit_mgL, FRP_mgL, ... {phytoplankton  
↪ placeholder/s}
```

With regard to the above **BC Header ==** command:

- DO_mgL, Si_mgL, Amm_mgL, Nit_mgL and FRP_mgL are the headers used to designate oxygen, silicate, ammonium, nitrate and FRP in the related boundary condition file, respectively
- Whilst this ordering in the command is fixed, the corresponding columnar data can appear in any order in the associated boundary condition file
- The header texts “DO_mgL”, “Si_mgL”, “Amm_mgL”, “Nit_mgL” and “FRP_mgL” are not special keywords. They can be any headers desired, as long as they match the correct respective boundary condition file column headers

4.7.5.1.2 Phosphorus model FRPhsads

If adsorbed FRP is simulated (i.e. **Phosphorus Model == FRPhsads**), then in all columnar and list style initial conditions, computed variables are expected in the following order (and map to “wq_1” etc accordingly):

Initial WQ Concentration == [DO], [Si], [NH₄], [NO₃], [FRP], [FRPads], ... {phytoplankton placeholder/s}

Similarly, in a **BC Header ==** command within a BC block, the following order of computed variables is expected after hydrodynamic boundary conditions:

BC Header == {HD BCs} ... DO_mgL, Si_mgL, Amm_mgL, Nit_mgL, FRP_mgL, FRP_ads_mgL, ...
 ↳ phytoplankton placeholder/s

With regard to the above **BC Header ==** command:

- DO_mgL, Si_mgL, Amm_mgL, Nit_mgL, FRP_mgL and FRP_ads_mgL are the headers used to designate oxygen, silicate, ammonium, nitrate, FRP and adsorbed FRP in the related boundary condition file, respectively
- Whilst this ordering in the command is fixed, the corresponding columnar data can appear in any order in the associated boundary condition file
- The header texts “DO_mgL”, “Si_mgL”, “Amm_mgL”, “Nit_mgL”, “FRP_mgL” and “FRP_ads_mgL” are not special keywords. They can be any headers desired, as long as they match the correct respective boundary condition file column headers

4.7.5.2 Including phytoplankton

Phytoplankton initial conditions and “**BC Header ==**” fields are appended directly to the above computed variable specifications, as denoted by the {phytoplankton placeholder/s} flag above.

Each phytoplankton group is specified using a cluster of values (initial conditions) or headers (BC block) and these clusters must appear in the same order as phytoplankton groups are specified in the water quality control file. The content of each phytoplankton cluster is determined both by the phytoplankton constituent model used and the settling model selected. These are described below, using a placeholder for preceding (non-phytoplankton) computed variables for clarity. These are described above and can be interpreted as either of the orderings specified in Section 4.7.5.1.1 or Section 4.7.5.1.2.

Two phytoplankton groups are used in all examples.

4.7.5.2.1 Basic phytoplankton model

If the basic phytoplankton constituent model is used, then in all columnar and list style initial conditions, computed variables are expected in the following order (and map to “wq_xx” after the final computed variable number accordingly):

Initial WQ Concentration == {non-phytoplankton placeholders} ... $\frac{PHY_1}{\text{Cluster 1}}$, $\frac{PHY_2}{\text{Cluster 2}}$

In order to match water quality control file groups with initial conditions, it is assumed that the groups’ clusters of initial conditions are specified above in the same order that **Phyto Model ==** blocks are presented in the water quality control file.

Similarly, in a **BC Header ==** command within a BC block, the following order of computed variables is expected after hydrodynamic and non-phytoplankton boundary conditions:

BC Header == {HD BCs} ... {non-phytoplankton placeholders} ... $\frac{\text{phyto_green}}{\text{Cluster 1}}$, $\frac{\text{phyto_bluegreen}}{\text{Cluster 2}}$

With regard to the above **BC Header ==** command:

- phyto_green and phyto_bluegreen are the headers used to designate the boundary concentrations of the two phytoplankton groups listed in the water quality control file
- In order to match water quality control file groups with these boundary condition clusters, it is assumed that the groups’ boundary condition header clusters are specified above in the same order that **Phyto Model ==** blocks appear in the water quality control file
- Although the names listed in the **BC Header ==** command above do not need to match the names listed in the water quality control file phytoplankton blocks, it is recommended that they do have names that are correlated with the phytoplankton group names in the water quality control file, for model integrity

- Whilst this ordering in the command is fixed, the corresponding columnar data can appear in any order in the associated boundary condition file
- The header texts “phyto_green” and “phyto_bluegreen” are not special keywords. They can be any headers desired, as long as they match the correct respective boundary condition file column headers

If the command `Settling == Stokes` is used for a phytoplankton group, then phytoplankton cell density must be simulated as a computed variable that requires initial and boundary conditions. This therefore affects the clustering of phytoplankton initial and boundary conditions. For example, if the first (and not the second) phytoplankton group above used the stokes settling model, then the following initial condition command would be required:

`Initial WQ Concentration == {HD} ... {non-phytoplankton placeholders} ...  $\underbrace{[PHY_1], \rho_{phy1}}_{\text{Cluster 1}}, \underbrace{[PHY_2]}_{\text{Cluster 2}}$`

ρ_{phy1} is the initial density of the first phytoplankton group’s cells. A density initial condition is not required for the second phytoplankton species because it does not use stokes settling.

Similarly, in a `BC Header ==` command within a BC block, the following order of computed variables is expected after hydrodynamic and non-phytoplankton boundary conditions:

`BC Header == {HD BCs} ... {non-phytoplankton placeholders} ...  $\underbrace{\text{phyto\_green, phyto\_green\_density}}_{\text{Cluster 1}}, \underbrace{\text{phyto\_bluegreen}}_{\text{Cluster 2}}$`

If both phytoplankton groups simulated density then the corresponding initial condition and boundary condition commands would be as follows:

`Initial WQ Concentration == {HD} ... {non-phytoplankton placeholders} ...  $\underbrace{[PHY_1], \rho_{phy1}}_{\text{Cluster 1}}, \underbrace{[PHY_2], \rho_{phy2}}_{\text{Cluster 2}}$`

`BC Header == {HD BCs} ... {non-phytoplankton placeholders} ...  $\underbrace{\text{phyto\_green, phyto\_green\_density}}_{\text{Cluster 1}}, \underbrace{\text{phyto\_bluegreen, phyto\_bluegreen\_density}}_{\text{Cluster 2}}$`

ρ_{phy1} and ρ_{phy2} are the initial densities of the first and second phytoplankton group’s cells.

The same notes provided above apply to these commands.

4.7.5.2.2 Advanced phytoplankton model

If the advanced phytoplankton constituent model is used, then in all columnar and list style initial conditions, computed variables are expected in the following order (and map to “WQ_XX” after the final computed variable number accordingly):

`Initial WQ Concentration == {non-phytoplankton placeholders} ...  $\underbrace{[PHY_1], [IN_1], [IP_1]}_{\text{Cluster 1}}, \underbrace{[PHY_2], [IN_2], [IP_2]}_{\text{Cluster 2}}$`

In order to match water quality control file groups with initial conditions, it is assumed that the groups’ initial conditions are specified above in the same order that `Phyto Model ==` blocks are presented in the water quality control file.

Similarly, in a `BC Header ==` command within a BC block, the following order of computed variables is expected after hydrodynamic and non-phytoplankton boundary conditions:

`BC Header == {HD BCs} ... {non-phytoplankton placeholders} ...  $\underbrace{\text{phyto\_gr, gr\_intN, gr\_intP}}_{\text{Cluster 1}}, \underbrace{\text{phyto\_blgr, blgr\_intN, blgr\_intP}}_{\text{Cluster 2}}$`

With regard to the above `BC Header ==` command:

- phyto_gr and phyto_blgr are the headers used to designate the boundary concentrations of the two phytoplankton groups listed in the water quality control file
- gr_intN and gr_intP are the headers used to designate the boundary concentrations of internal nitrogen and internal phosphorus for the green phytoplankton group, respectively
- blgr_intN and blgr_intP are the headers used to designate the boundary concentrations of internal nitrogen and internal phosphorus for the bluegreen group, respectively
- In order to match water quality control file groups with these boundary conditions, it is assumed that the groups’ boundary condition header clusters are specified above in the same order that `Phyto Model ==` blocks appear in the water quality control file
- Although the names listed in the `BC Header ==` command above do not need to match the names listed in the water quality control file phytoplankton blocks, it is recommended that they do have names that are correlated with the phytoplankton group names in the water quality control file, for model integrity
- Whilst this ordering in the command is fixed, the corresponding columnar data can appear in any order in the associated boundary condition file

- The header texts “phyto_gr” and “phyto_blgr” are not special keywords. They can be any headers desired, as long as they match the correct respective boundary condition file column headers

If the command `Settling == Stokes` is used for a phytoplankton group, then phytoplankton cell density must be simulated as a computed variable that requires initial and boundary conditions. This therefore affects the clustering of phytoplankton initial and boundary conditions. If the first phytoplankton group above used the advanced phytoplankton model with the stokes settling model, and the second group used the basic phytoplankton model without stokes settling, then the following commands would be required:

```
Initial WQ Concentration == {non-phytoplankton placeholders} ...  $\underbrace{[PHY_1], \rho_{phy1}, [IN_1], [IP_1]}_{\text{cluster 1}}, \underbrace{[PHY_2]}_{\text{cluster 2}}$ 
```

Similarly, in a `BC Header ==` command within a BC block, the following order of computed variables is expected after hydrodynamic and non-phytoplankton boundary conditions:

```
BC Header == {HD BCs} ... {non-phytoplankton placeholders} ...  $\underbrace{\text{phyto\_gr, gr\_dens, gr\_intN, gr\_intP}}_{\text{cluster 1}},$   
 $\underbrace{\text{phyto\_blgr}}_{\text{cluster 2}}$ 
```

If both phytoplankton groups simulated density, again with the first and second groups using the advanced and basic models respectively, then the corresponding commands would be as follows:

```
Initial WQ Concentration == {non-phytoplankton placeholders} ...  $\underbrace{[PHY_1], \rho_{phy1}, [IN_1], [IP_1]}_{\text{cluster 1}}, \underbrace{[PHY_2], \rho_{phy2}}_{\text{cluster 2}}$   
BC Header == {HD BCs} ... {non-phytoplankton placeholders} ...  $\underbrace{\text{phyto\_gr, gr\_dens, gr\_intN, gr\_intP}}_{\text{cluster 1}},$   
 $\underbrace{\text{phyto\_blgr, blgr\_dens}}_{\text{cluster 2}}$ 
```

The same notes provided above apply to these commands.

4.7.5.3 Including pathogens (optional)

The ordering requirements for pathogens are the same as those described in Section 4.6.5.1. Pathogen headers are always included last (i.e. after phytoplankton in the inorganics simulation class).

4.7.6 Example

Following is an example of all the available WQ Module `Simulation Class == Inorganics` commands, with a single material applied as zeros everywhere as the default, and then modified by a further specification for materials 3 and 7. Two phytoplankton groups (one each of the basic and advanced models) are set. Pathogens have been omitted for clarity, but could be added as per Section 4.6.6.

Example - `Simulation Class == Inorganics`

```
Simulation Class == Inorganics  
WQ dt == 3600  
WQ Units == mgL  
  
Oxygen Model == O2  
    Oxygen Benthic == 4.0, 1.05  
    Oxygen Min Max == 0.0, 25.0  
End Oxygen Model  
  
Silicate Model == Si  
    Silicate Benthic == 4.0, 1.05  
    Silicate Min Max == 0.0, 2500.0  
    Oxygen == ON  
End Silicate Model  
  
Inorganic Nitrogen Model == AmmoniumNitrate  
    Ammonium Benthic == 4.0, 1.05  
    Nitrate Benthic == 4.0, 1.05
```

```

    Ammonium Min Max == 0.0, 50.0
    Nitrate Min Max == 0.0, 110.0
    Nitrification == 0.1, 4.0, 1.05
    Denitrification == Exponential, 0.5, 8.0, 1.05
    Atmospheric Deposition == 10.0, 2.4, 0.15
    Oxygen == ON
End Inorganic Nitrogen Model

Inorganic Phosphorus Model == FRPhsAds
    FRP Benthic == 4.0, 1.05
    FRP Min Max == 0.0, 50.0
    FRPads Min Max == 0.0, 50.0
    Atmospheric Deposition == 5.0, 1.4
    Adsorption == Quadratic, 1.5, 0.5
    Settling == 0.000001
    Oxygen == ON
End Inorganic Phosphorus Model

Phyto Model == Basic, Green
    Min Max == 0.01, 40.0
    Temperature Limitation == Standard, 11.0, 14.0, 30.0
    Salinity Limitation == None
    Light Limitation == Monod, 0.3, 70.0
    Settling == Constant, 0.01
    Nitrogen Limitation == 0.01, 1.5
    Phosphorus Limitation == 0.001, 0.03
    Silicate Limitation == 0.5, 7.0
    Uptake == 4.7, 0.6, 8.9
    Carbon Chla Ratio == 32.0
    Primary Productivity == 2.0, 1.06
    Respiration == 0.02, 1.04, 0.1, 0.05, 0.6
End Phyto Model

Phyto Model == Advanced, Bluegreen
    Min Max == 0.5, 50.0
    Temperature Limitation == Standard, 10.0, 15.0, 25.0
    Salinity Limitation == Estuarine, 22.0, 35.0, 0.0
    Light Limitation == Monod, 0.5, 51.0
    Settling == Motile, 0.5
    Nitrogen Limitation == 0.05, 2.5, 4.0, 5.0
    Phosphorus Limitation == 0.01, 0.05, 0.64, 0.67
    Silicate Limitation == 1.0, 5.0
    Uptake == 0.05, 0.05, 8.9
    Carbon Chla Ratio == 27.0
    Nitrogen Fixing == 0.100, 0.100
    Primary Productivity == 1.0, 1.08
    Respiration == 0.01, 1.01, 0.2, 0.0, 0.4
End Phyto Model

Material == Default
    Oxygen Flux == 0.0
    Silicate Flux == 0.0
    Ammonium Flux == 0.0
    Nitrate Flux == 0.0
    FRP Flux == 0.0
End Material

Material == 3, 7
    Oxygen Flux == -800.0
    Silicate Flux == 122.0
    Ammonium Flux == 37.0
    Nitrate Flux == 3.7
    FRP Flux == 1.4

```

End Material

4.8 Simulation Class: Organics

If the organics simulation class is specified with no subsequent constituent model blocks, then a simulation will be automatically constructed using this organics class, and populated with library defaults for all parameters. Computed variables will be:

- Dissolved oxygen
- Silicate
- Ammonium
- Nitrate
- Filterable reactive phosphorus
- Dissolved organic carbon
- Particulate organic carbon
- Dissolved organic nitrogen
- Particulate organic nitrogen
- Dissolved organic phosphorus
- Particulate organic phosphorus
- One phytoplankton group named 'dummy' that uses the basic phytoplankton constituent model

For clarity, this section uses acronyms for some computed variable names, and these acronyms are expanded in Appendix O. All references below to “organic matter” are to labile organic computed variables, unless specifically termed as refractory.

4.8.1 Prerequisites

The organics simulation class requires simulation of the following in TUFLOW FV:

- Hydrodynamics, in either two or three dimensions (including any internal one dimensional structures if present)
- Salinity
- Temperature
- Heat module on (i.e. meteorological forcing is required)

Simulation of suspended sediment (via TUFLOW FV's sediment transport module) is required only if adsorbed phosphorus is to be simulated by the WQ Module.

4.8.2 Part 1: Simulation specification

The organics simulation class is set via

```
Simulation Class == Organics
```

The other commands in this part are not specific to this simulation class. See Section 4.5.1.

4.8.3 Part 2: Constituent model specification

As per Table 2.2 and Table 2.3, there are several constituent model classes available within the organics simulation class. The commands for each are described following. To avoid repetition, cross references to explanations are provided for commands that are included in previous simulation classes and remain the same for this class.

4.8.3.1 Model class: Oxygen

4.8.3.1.1 Constituent model: O2

The commands for this constituent model are described in Section 4.7.3.1.1.

4.8.3.2 Model class: Silicate

4.8.3.2.1 Constituent model: Si

The commands for this constituent model are described in Section 4.7.3.2.1.

4.8.3.3 Model class: Inorganic nitrogen

4.8.3.3.1 Constituent model: AmmoniumNitrate

The commands for this constituent model are described in Section 4.7.3.3.1.

4.8.3.4 Model class: Inorganic phosphorus

4.8.3.4.1 Constituent model: FRPhs

The commands for this constituent model are described in Section 4.7.3.4.1.

4.8.3.4.2 Constituent model: FRPhsAds

The commands for this constituent model are described in Section 4.7.3.4.2.

4.8.3.5 Model class: Organic matter

4.8.3.5.1 Constituent model: Labile

This constituent model is specified as:

`Organic Matter Model == Labile`

Minimum and maximum concentrations are specified as:

`Carbon Min Max == [POC]minPOC, [POC]maxPOC, [DOC]minDOC, [DOC]maxDOC`

`Nitrogen Min Max == [PON]minPON, [PON]maxPON, [DON]minDON, [DON]maxDON`

`Phosphorus Min Max == [POP]minPOP, [POP]maxPOP, [DOP]minDOP, [DOP]maxDOP`

Global benthic flux parameters (used in Equation M.1) are specified as:

`organics Benthic ==  $K_{sed-O_2}^{DOM}$ ,  $\theta_{sed}^{DOM}$`

Although not strictly necessary, the use of “organics” to prefix the above block command is deliberate so as to maintain consistency of command style with other constituent model blocks that include more than one computed variable, such as nitrogen and phosphorus. The command will also be accepted simply as `Benthic ==`.

Particulate organic hydrolysis parameters (used in Equation M.2 and therefore Equation M.3) are set in a single command as:

`Hydrolysis ==  $R_{hyd}^{POC}$ ,  $R_{hyd}^{PON}$ ,  $R_{hyd}^{POP}$ ,  $K_{hyd-O_2}^{POM}$ ,  $\theta_{hyd}^{POM}$`

Dissolved organic mineralisation parameters (used in Equation M.8 and therefore Equation M.9) are set in a single command, together with the corresponding denitrification parameters describing associated consumption of nitrate due to mineralisation (used in Equation M.10 and Equation M.14) as:

`Mineralisation ==  $R_{miner}^{DOM}$ ,  $K_{miner-O_2}^{DOM}$ ,  $\theta_{miner}^{DOM}$ ,  $f_{an}$ ,  $K_{miner-NO_3}^{NO_3}$`

If $K_{miner-NO_3}^{NO_3}$ is set to 0.0, then the consumption of nitrate due to mineralisation of organic matter is switched off.

Settling of labile particulate organic matter can be specified by one of the following models:

- None

`Settling == None`

or

- Constant

`Settling == Constant,  $V_{settle}^{lorg}$`

or

- Constant with density correction (as per Equation M.28)

`Settling == Thermal,  $V_{settle}^{lorg}$`

or

- Stokes (used in Equation M.29)

`Settling == Stokes,  $d_{lorg}$ ,  $\rho_{lorg}$`

Self shading due to the presence of labile organics (used in Equation M.26) parameters are set as:

`Self Shading ==  $Ke^{POM}$ ,  $Ke^{DOM}$`

This constituent model block must be terminated using the command:

`End Organic Matter Model`

4.8.3.5.2 Constituent model: Refractory

This constituent model encompasses all the functionality (and commands) of the labile organic matter constituent model, but offers further commands to simulate refractory organic processes, and their interaction with labile organic and inorganic computed variables.

This constituent model is specified as:

`Organic Matter Model == Refractory`

Minimum and maximum concentrations are specified as follows. The carbon command includes the specification of refractory particulate organic matter minimums and maximums, as well as dissolved refractories.

`Ref Carbon Min Max ==  $[RPOM]_{min}^{RPOM}$ ,  $[RPOM]_{max}^{RPOM}$ ,  $[RDOC]_{min}^{RDOC}$ ,  $[RDOC]_{max}^{RDOC}$`

`Ref Nitrogen Min Max ==  $[RDON]_{min}^{RDON}$ ,  $[RDON]_{max}^{RDON}$`

`Ref Phosphorus Min Max ==  $[RDOP]_{min}^{RDOP}$ ,  $[RDOP]_{max}^{RDOP}$`

The breakdown of refractory particulate organic matter into labile particulate organic matter (used in Equation M.5 and Equation M.6) parameters are set as:

`Ref Breakdown ==  $R_{bdn}^{RPOM}$ ,  $X_N^{RPOM}$ ,  $X_P^{RPOM}$`

The activation of refractory dissolved organic matter to labile dissolved organic matter (used in Equation M.17 and Equation M.18) parameter is set as:

`Ref Activation ==  $R_{act}^{RDOM}$`

The photolysis of refractory organics (used in Equation M.27) is not turned on unless the following command is issued. It sets the parameter that proportions the split of photolysed refractory dissolved organics to labile dissolved organics and inorganics:

`Ref Photolysis ==  $f_{photo}^{RDOM}$`

Settling of refractory particulate organic matter can be specified by one of the following models:

- None

`Ref Settling == None`

or

- Constant

`Ref Settling == Constant,  $V_{settle}^{rorg}$`

or

- Constant with density correction (as per Equation M.28)

`Ref Settling == Thermal,  $V_{settle}^{rorg}$`

or

- Stokes (used in Equation M.29)

`Ref Settling == Stokes,  $d_{rorg}$ ,  $\rho_{rorg}$`

The settling model selected for the refractory particulate organic matter model must be the same as that of the labile particulate organic matter. The input parameters to this model may be different.

Self shading due to the presence of refractory organics (used in Equation M.27) parameters are set as:

`Ref Self Shading ==  $Ke^{RPOM}$ ,  $R_{CDOM}^{RDOM}$`

This constituent model block must be terminated using the command:

`End Organic Matter Model`

4.8.3.6 Model class: Phytoplankton

4.8.3.6.1 Constituent model: Basic

The commands for this constituent model are described in Section 4.7.3.5.1.

4.8.3.6.2 Constituent model: Advanced

The commands for this constituent model are described in Section 4.7.3.5.2.

4.8.3.7 Model class: Pathogens (optional)

This model class is optional.

4.8.3.7.1 Constituent model: Free

The commands for this constituent model are described in Section 4.6.3.2.1.

4.8.3.7.2 Constituent model: Attached

The commands for this constituent model are described in Section 4.6.3.2.2.

4.8.4 Part 3: Material specification

Oxygen, silicate, ammonium, nitrate FRP, dissolved organic carbon, dissolved organic nitrogen and dissolved organic phosphorus benthic fluxes are specified within both default and numbered material blocks as:

Oxygen Flux == $F_{sed}^{O_2}$
 Silicate Flux == F_{sed}^{sil}
 Ammonium Flux == $F_{sed}^{NH_4}$
 Nitrate Flux == $F_{sed}^{NO_3}$
 FRP Flux == F_{sed}^{FRP}
 DOC Flux == F_{sed}^{DOC}
 DON Flux == F_{sed}^{DON}
 DOP Flux == F_{sed}^{DOP}

No adsorbed FRP, phytoplankton or particulate organic fluxes are required.

4.8.5 Constituent ordering

As for the inorganics simulation class (see Section 4.7.5) different organic matter constituent model selections require different orderings in specifying computed variable initial conditions and `BC Header ==` commands. Notwithstanding this, all the ordering information presented in Section 4.7.5 for the inorganics simulation class applies equally to the

organics simulation class, other than for insertions related to the simulation of organics (described below). As such, that section should be reviewed with regard to ordering of the following:

- Dissolved oxygen
- Silicate
- Inorganic nitrogen
- Inorganic phosphorus (including the optional simulation of adsorbed FRP), and
- Phytoplankton groups (including the basic and advanced phytoplankton constituent models, with and without simulation of cell density)

The additional initial condition and **BC Header ==** fields related to the organics simulation class do not change the order of computed variable fields presented in Section 4.7.5 other than to insert organic matter constituent model computed variables immediately after FRP computed variables and immediately prior to required phytoplankton fields. This insertion and ordering is presented following for the labile and refractory organic matter constituent models.

4.8.5.1 Labile

The computed variables required to be specified within the labile organic matter constituent model are, in order:

- Dissolved organic carbon
- Particulate organic carbon
- Dissolved organic nitrogen
- Particulate organic nitrogen
- Dissolved organic phosphorus
- Particulate organic phosphorus

All columnar and list style initial condition computed variables are therefore expected in the following order (and map to “wq_1” etc accordingly)

Initial WQ Concentration == [DO], [Si], [NH₄], [NO₃], [FRP], (optionally [FRPads]), [DOC], [POC], [DON], [PON], [DOP], [POP], ... {phytoplankton placeholder/s}

Similarly, in a **BC Header ==** command within a BC block, the following order of computed variables is expected after hydrodynamic (HD BCs) boundary conditions (and map to “wq_1” etc accordingly):

BC Header == {HD BCs} ... DO_mgL, Si_mgL, Amm_mgL, Nit_mgL, FRP_mgL, (optionally FRPads_mgL), DOC_mgL, POC_mgL, DON_mgL, PON_mgL, DOP_mgL, POP_mgL, ... {phytoplankton placeholder/s}

With regard to the above **BC Header ==** command:

- DO_mgL, Si_mgL, Amm_mgL, Nit_mgL, FRP_mgL (optionally FRPads_mgL), DOC_mgL, POC_mgL, DON_mgL, PON_mgL, DOP_mgL and POP_mgL are the headers used to designate oxygen, silicate, ammonium, nitrate, FRP (optionally adsorbed FRP), dissolved organic carbon, particulate organic carbon, dissolved organic nitrogen, particulate organic nitrogen, dissolved organic phosphorus and particulate organic phosphorus in the related boundary condition file, respectively
- Whilst this ordering in the command is fixed, the corresponding columnar data can appear in any order in the associated boundary condition file
- The header texts “DO_mgL”, “Si_mgL”, “Amm_mgL”, “Nit_mgL”, “FRP_mgL” (optionally “FRPads_mgL”), “DOC_mgL”, “POC_mgL”, “DON_mgL”, “PON_mgL”, “DOP_mgL” and “POP_mgL” are not special keywords. They can be any headers desired, as long as they match the correct respective boundary condition file column headers

4.8.5.2 Refractory

The computed variables required to be specified within the labile organic matter constituent model are, in order:

- Dissolved organic carbon
- Particulate organic carbon
- Dissolved organic nitrogen
- Particulate organic nitrogen
- Dissolved organic phosphorus
- Particulate organic phosphorus
- Refractory dissolved organic carbon
- Refractory dissolved organic nitrogen

- Refractory dissolved organic phosphorus
- Refractory particulate organic matter

All columnar and list style initial condition computed variables are therefore expected in the following order (and map to “wq_1” etc accordingly)

Initial WQ Concentration == [DO], [Si], [NH₄], [NO₃], [FRP], (optionally [FRPads]), [DOC], [POC], [DON], [PON], [DOP], [POP], [RDOC], [RDON], [RDOP], [RPOM], ... {phytoplankton placeholder/s}

Similarly, in a **BC Header** == command within a BC block, the following order of computed variables is expected after hydrodynamic (HD BCs) boundary conditions (and map to “wq_1” etc accordingly):

BC Header == {HD BCs} ... DO_mgL, Si_mgL, Amm_mgL, Nit_mgL, FRP_mgL, (optionally FRPads_mgL), DOC_mgL, POC_mgL, DON_mgL, PON_mgL, DOP_mgL, POP_mgL, RDOC_mgL, RDON_mgL, RDOP_mgL, RPOM_mgL, ... {phytoplankton placeholder/s}

With regard to the above **BC Header** == command:

- DO_mgL, Si_mgL, Amm_mgL, Nit_mgL, FRP_mgL (optionally FRPads_mgL), DOC_mgL, POC_mgL, DON_mgL, PON_mgL, DOP_mgL, POP_mgL, RDOC_mgL, RDON_mgL, RDOP_mgL and RPOM_mgL are the headers used to designate oxygen, silicate, ammonium, nitrate, FRP (optionally adsorbed FRP), dissolved organic carbon, particulate organic carbon, dissolved organic nitrogen, particulate organic nitrogen, dissolved organic phosphorus, particulate organic phosphorus, refractory dissolved organic carbon, refractory dissolved nitrogen, refractory dissolved phosphorus and refractory particulate organic matter in the related boundary condition file, respectively
- Whilst this ordering in the command is fixed, the corresponding columnar data can appear in any order in the associated boundary condition file
- The header texts “DO_mgL”, “Si_mgL”, “Amm_mgL”, “Nit_mgL”, “FRP_mgL” (optionally “FRPads_mgL”), “DOC_mgL”, “POC_mgL”, “DON_mgL”, “PON_mgL”, “DOP_mgL”, “POP_mgL”, “RDOC_mgL”, “RDON_mgL”, “RDOP_mgL” and “RPOM_mgL” are not special keywords. They can be any headers desired, as long as they match the correct respective boundary condition file column headers.

4.8.5.3 Including pathogens (optional)

The ordering requirements for pathogens are the same as those described in Section 4.6.5.1. Pathogen headers are always included last (i.e. after phytoplankton in the organics simulation class).

4.8.6 Example

Following is an example of all the available WQ Module **Simulation Class** == organics commands, with a single material applied as zeros everywhere as the default, and then modified by a further specification for materials 3 and 7. Two phytoplankton groups (one each of the basic and advanced models) are set, and the refractory organic matter constituent model deployed. Pathogens have been omitted for clarity, but could be added as per Section 4.6.6.

Example - **Simulation Class** == organics

```
Simulation Class == Organics
WQ dt == 900
WQ Units == mgL

Oxygen Model == O2
    Oxygen Benthic == 4.0, 1.05
    Oxygen Min Max == 0.0, 25.0
End Oxygen Model

Silicate Model == Si
    Silicate Benthic == 4.0, 1.05
    Silicate Min Max == 0.0, 2500.0
    Oxygen == ON
End Silicate Model

Inorganic Nitrogen Model == AmmoniumNitrate
```

```

Ammonium Benthic == 4.0, 1.05
Nitrate Benthic == 4.0, 1.05
Ammonium Min Max == 0.0, 50.0
Nitrate Min Max == 0.0, 50.0
Nitrification == 0.1, 4.0, 1.05
Denitrification == Exponential, 0.5, 8.0, 1.05
Atmospheric Deposition == 10.0, 2.4, 0.15
Oxygen == ON
End Inorganic Nitrogen Model

Inorganic Phosphorus Model == FRPhsAds
FRP Benthic == 4.0, 1.05
FRP Min Max == 0.0, 35.0
FRPads Min Max == 0.0, 35.0
Atmospheric Deposition == 5.0, 1.4
Adsorption == Quadratic, 1.5, 0.5
Oxygen == ON
End Inorganic Phosphorus Model

Phyto Model == Basic, Green
Min Max == 0.01, 40.0
Temperature Limitation == Standard, 11.0, 14.0, 30.0
Salinity Limitation == None
Light Limitation == Monod, 0.3, 70.0
Settling == Constant, 0.01
Nitrogen Limitation == 0.01, 1.5
Phosphorus Limitation == 0.001, 0.03
Silicate Limitation == 0.5, 7.0
Uptake == 4.7, 0.6, 8.9
Carbon Chla Ratio == 32.0
Primary Productivity == 2.0, 1.06
Respiration == 0.02, 1.04, 0.1, 0.05, 0.6
End Phyto Model

Phyto Model == Advanced, Bluegreen
Min Max == 0.5, 50.0
Temperature Limitation == Standard, 10.0, 15.0, 25.0
Salinity Limitation == Estuarine, 22.0, 35.0, 0.0
Light Limitation == Monod, 0.5, 51.0
Settling == Motile, 0.5
Nitrogen Limitation == 0.05, 2.5, 4.0, 5.0
Phosphorus Limitation == 0.01, 0.05, 0.64, 0.67
Silicate Limitation == 1.0, 5.0
Uptake == 0.05, 0.05, 8.9
Carbon Chla Ratio == 27.0
Nitrogen Fixing == 0.100, 0.100
Primary Productivity == 1.0, 1.08
Respiration == 0.01, 1.01, 0.2, 0.0, 0.4
End Phyto Model

Organic Matter Model == Refractory
Carbon Min Max == 0.0, 35.0, 0.0, 35.0, 0.0, 50.0
Nitrogen Min Max == 0.0, 25.0, 0.0, 25.0
Phosphorus Min Max == 0.0, 5.0, 0.0, 5.0
Organics Benthic == 4.5, 1.03
Hydrolysis == 1.2, 0.19, 0.031, 4.2, 1.1
Mineralisation == 0.053, 4.1, 1.02, 0.6, 1.2
Self Shading == 0.0003, 0.00025
Ref Carbon Min Max == 0.0, 40.0, 0.0, 35.0
Ref Nitrogen Min Max == 0.0, 25.0
Ref Phosphorus Min Max == 0.0, 5.0
Ref Breakdown == 0.002, 0.15, 0.0094
Ref Activation == 0.02

```

```

    Ref Photolysis == 0.03
    Ref Self Shading == 0.00031, 0.00022
End Organic Matter Model

Material == Default
    Oxygen Flux == 0.0
    Silicate Flux == 0.0
    Ammonium Flux == 0.0
    Nitrate Flux == 0.0
    FRP Flux == 0.0
    DOC Flux == 0.0
    DON Flux == 0.0
    DOP Flux == 0.0
End Material

Material == 3, 7
    Oxygen Flux == -400.0
    Silicate Flux == 12.0
    Ammonium Flux == 33.0
    Nitrate Flux == 3.7
    FRP Flux == 1.4
    DOC Flux == 12.0
    DON Flux == 1.81
    DOP Flux == 0.29
End Material

```

4.9 Outputs

WQ Module outputs are set via commands specified in the TUFLOW FV control file, as described below. Available outputs include:

- WQ Module outputs:
 - Computed variables, i.e. time varying concentrations of simulated quantities (e.g. dissolved oxygen). See [Appendix O](#)
 - Diagnostic variables, i.e. time varying quantities that describe rates, and similar such processes which modify computed variables (e.g. sediment flux of nitrate). See [Appendix P](#)
- TUFLOW FV integrated outputs of WQ Module variables:
 - Fluxes across predefined nodestrings, e.g. the time varying flux of a WQ Module computed variable integrated by TUFLOW FV across a two dimensional vertical curtain, and
 - Instantaneous masses, e.g. the time varying integrated mass of a WQ Module computed variable, computed across the entire model domain
 - Mass balance fluxes, .e.g. the cumulative flux of mass through:
 - * Every water quality flux pathway (such as oxygen production due to a phytoplankton group's primary productivity), and
 - * Every QC, QC_POLY, Q, WL, WLS and QN boundary

Computed and diagnostic variables are output directly by the WQ Module, whilst integrated outputs are computed by TUFLOW FV, using WQ Module computed and diagnostic variables as inputs.

All these types of outputs use the same structures as described in the TUFLOW FV user manual for hydrodynamic and other TUFLOW FV outputs, namely via specification of `output ==` blocks. The relevant sections of the TUFLOW FV manual should be reviewed to supplement the material presented here. WQ Module and TUFLOW FV outputs are described below.

4.9.1 WQ Module outputs

All WQ Module output computed and diagnostic variables, together with their output names, are included in Appendices [Appendix O](#) and [Appendix P](#). The listed output names can be copied and pasted directly from the Appendices to a control file, with the exception of phytoplankton variables, where the user specified group name is included within the variable name, so will need to be inserted by the user.

The most common `Output ==` blocks used by the WQ Module to report the time variation of computed and/or diagnostic variables are:

- 0D points: `Output == Points` (these are depth averaged timeseries outputs at an X/Y location)
- 1D profiles: `Output == Profiles`
- 2D maps: `Output == DatV`
- 3D fields: `Output == NetCDF`

The simplest manner in which to specify the computed and diagnostic variables to be included in these blocks is to use the `WQ_A11` and `WQ_Diag_A11` flags against the `Output Parameters ==` command. An example of a 3D NetCDF output block that reports computed variables (`WQ_A11`) and diagnostic variables (`WQ_Diag_A11`) every hour is:

```
Output == NetCDF
  Output Parameters == WQ_A11, WQ_Diag_A11
  Output Interval == 3600.00
End Output
```

WQ Module outputs need not be in distinct output blocks of their own, but can be added to existing TUFLOW output blocks, for example:

```
Output == DatV
  Output Parameters == h, v, WQ_A11, WQ_Diag_A11
  Output Interval == 3600.00
  Vertical Averaging == Depth-A11
End Output
```

Water quality outputs are often voluminous. In order to avoid potentially cumbersome data handling issues around large output files, the `Output Parameters ==` command arguments can be tailored to list only those computed or diagnostic variables required for analysis, rather than using the blanket `WQ_A11` and `WQ_Diag_A11` arguments. An example of such an output command block that only reports dissolved oxygen concentration and atmospheric oxygen exchange is:

```
Output == NetCDF
  Output Parameters == h, WQ_DISS_OXYGEN_MG_L, WQ_DIAG_O2_ATMOS_EXCHANGE_MG_M2_D
  Output Interval == 3600.00
End Output
```

4.9.2 TUFLOW FV outputs

The most common `Output ==` blocks used to report the time variation of integrated quantities computed by TUFLOW FV are:

- Mass: `Output == Mass`
- Flux: `Output == Flux`
- Mass balance: `Output == Massbalance`

Variable names are not specified, with all available variables being included by default. Examples of such output blocks are:

```
Output == Mass
  Output Interval == 900.00
End Output
```

```
Output == Flux
  Output Interval == 900.00
End Output
```

```
Output == Massbalance
  Output Interval == 900.00
End Output
```

The first two output types produce one .csv file each, with headers that append ‘_MASS’ and ‘_FLUX’ to the variable names presented in the Appendices. The third `Massbalance` output is explained in detail in the TUFLOW FV documentation [here](#). In summary, this output produces:

- Mass fluxes in a single .csv file per water quality constituent, where each file contains timeseries of cumulative mass fluxes through every boundary and internal flux pathway relevant to that constituent

- Total cumulative mass fluxes (i.e. the sum of the above at each timestep)
- Multiple estimates of instantaneous mass (as timeseries) and associated percentage errors to allow for analysis of mass conservation performance
- Timeseries of the estimated number of mass turnovers of each water quality constituent (see link to TUFLOW FV documentation above for more detail), which assists in assessing the dynamism (i.e. rapidity of processing), of a constituent within the simulated domain

Across these automated outputs, users can interrogate the rate and manner in which each simulated quantity's mass is transformed through every relevant internal process (e.g. denitrification) and across every model boundary (e.g. tidal boundaries) within the simulated domain. These are referred to as 'mass fluxes', and this examination allows users to come to an understanding of the domain's overall environmental operation. This is separate and distinct to examining concentration timeseries at points (which is the traditional approach), which typically offers limited insight into system operation and can mask understanding if relied upon solely to assess model robustness. These flux outputs offered by TUFLOW FV are therefore valuable tools that assist in providing understanding as to *why* a model is predicting the water quality concentrations that it is, and so allow users to move beyond relying on concentration-based statistical assessments of model-to-measured data as a metric for model fitness for purpose. This understanding in turn shifts the potential pathway taken for model calibration and validation away from one that might include a degree of educated assumptions (and therefore large numbers of time consuming model reruns) and towards one that is evidence based with targeted and informed model parameter changes (and correspondingly less model reruns). As such, it is recommended strongly that these outputs be switched on as standard, and actively used across the entire water quality modelling calibration and scenario execution process.

Each simulated water quality constituent has its own .csv mass balance file written as an output, with relevant fluxes and masses. These can be opened directly in any spreadsheet package, plotted and/or reconfigured as a user wishes.

The following apply to the mass balance outputs produced by TUFLOW FV, as related to water quality simulation:

- Mechanics of outputs:
 - If adsorbed FRP is simulated, then its fluxes are reported together with FRP in the '...MASSBALANCE_WQ_FRP_MG_L.csv' file. This provides a complete description of FRP related mass fluxes in a single file. As such, the '...MASSBALANCE_WQ_FRP_ADS_MG_L.csv' file is created but not populated
 - Pathogen CFU fluxes are not reported. This is because typical CFU counts are very large numbers (1e+20 CFU is common) and the required mass balance calculations therefore suffer from not insignificant numerical truncation errors. This in turn leads to mass balances that relatively quickly become unstable. As such, the relevant '...MASSBALANCE_WQ_PATH_....csv' files are created but not populated
 - Mass balance of internal nutrients (i.e. use of the advanced phytoplankton model) is not supported
 - Mass balance of the MMM units system is not supported
 - Mass balance of nitrogen fixation is not supported
- Interpretation of outputs:
 - Mass should be conserved (generally) to within a few percent over an annual simulation period, for a given constituent. This depends significantly on the rates of change of all fluxes however, and where fluxes vary rapidly in time, mass balance errors should be expected to accumulate. One example of where this might be particularly relevant is across tidal boundaries where large tides in deep water occur - mass fluxes of water quality constituents will likely vary rapidly in these settings and cause potential mass balance reporting errors
 - Outputting mass balance csv files at a finer timestep may go part way to overcoming such error accumulation. However, if the output timestep is reduced too far, then some water quality processes will have fluxes so small that they are numerically truncated and written as zeros (when they are in fact non zero). This will cause additional mass balance errors, and these will compound in time
 - In order to provide value to a model set up and calibration process, focus should be given to concurrent examination of timeseries (for a given constituent) of:
 - ★ Total mass (computed from all methods),
 - ★ Cumulative mass fluxes, and
 - ★ Turnovers
 - This provides the simplest and cleanest overview of all mass fluxes and their relationship to total mass for a single computed variable - which in turn facilitates system understanding and provides direction to the selection of water quality parameters to alter in achieving calibration. This comparison should first be undertaken with volume, to elucidate water movement and turnover properties, and then on a constituent by constituent basis thereafter. An example for volume, dissolved oxygen and ammonium is presented below. It shows that:

- ★ Volume (Figure 4.2):
 - Water movement is dominated by catchment inflows (source) and tidal outflows (sink)
 - The system turns over water approximately 160 times in the period shown (orange line and secondary vertical axis)
- ★ Dissolved oxygen (Figure 4.3):
 - Dissolved oxygen's largest source is atmospheric aeration, and largest sinks are tidal outflow, sediment consumption and mineralisation of organics. Parameters that control these processes will therefore provide the greatest impact on model concentration predictions
 - The system turns over dissolved oxygen approximately 180 times in the period shown (orange line and secondary vertical axis) - this is 15% more rapid than the water turnover behaviour
- ★ Ammonium (Figure 4.4):
 - Ammonium's largest source in DRNA and largest sinks are tidal outflow and nitrification. Parameters that control these processes will therefore provide the greatest impact on model concentration predictions
 - The system turns over ammonium approximately 1000 times in the period shown (orange line and secondary vertical axis) - this is six times more rapid than the water turnover behaviour, and suggests that the system is highly dynamic with respect to ammonium and that perturbations may have non trivial impacts on system balance and resilience. This rapid rate of turnover is not evident from examining the total mass (or average concentration) alone, which is relatively steady over the simulation period. This points to the utility of examining mass fluxes at all times during a water quality modelling process, and not relying solely on concentration point-to-point comparisons

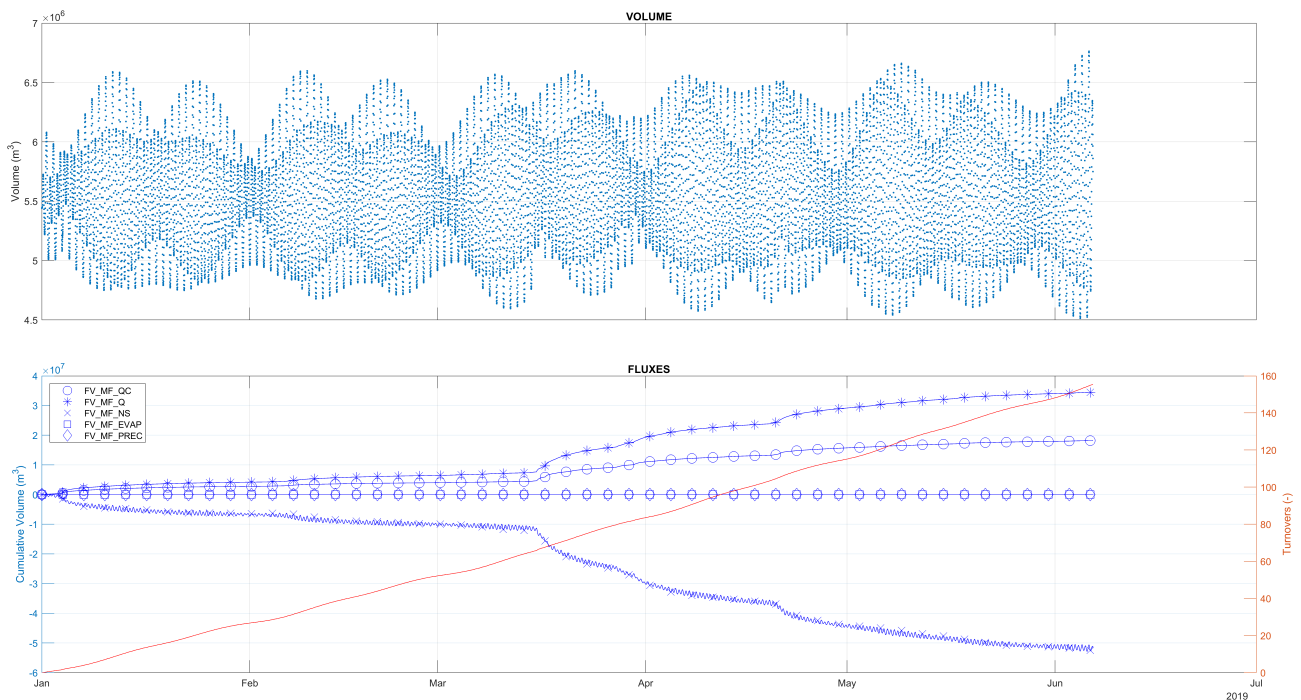


Figure 4.2: Mass balance output: Volume

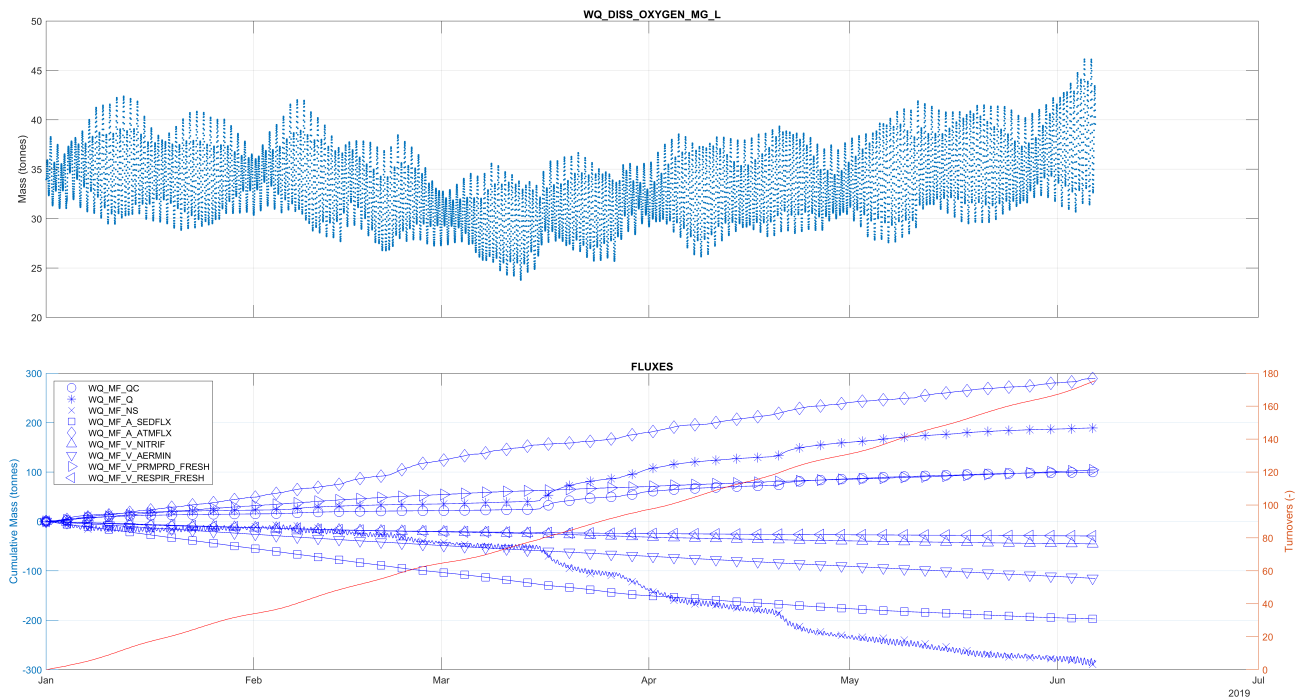


Figure 4.3: Mass balance output: Dissolved oxygen

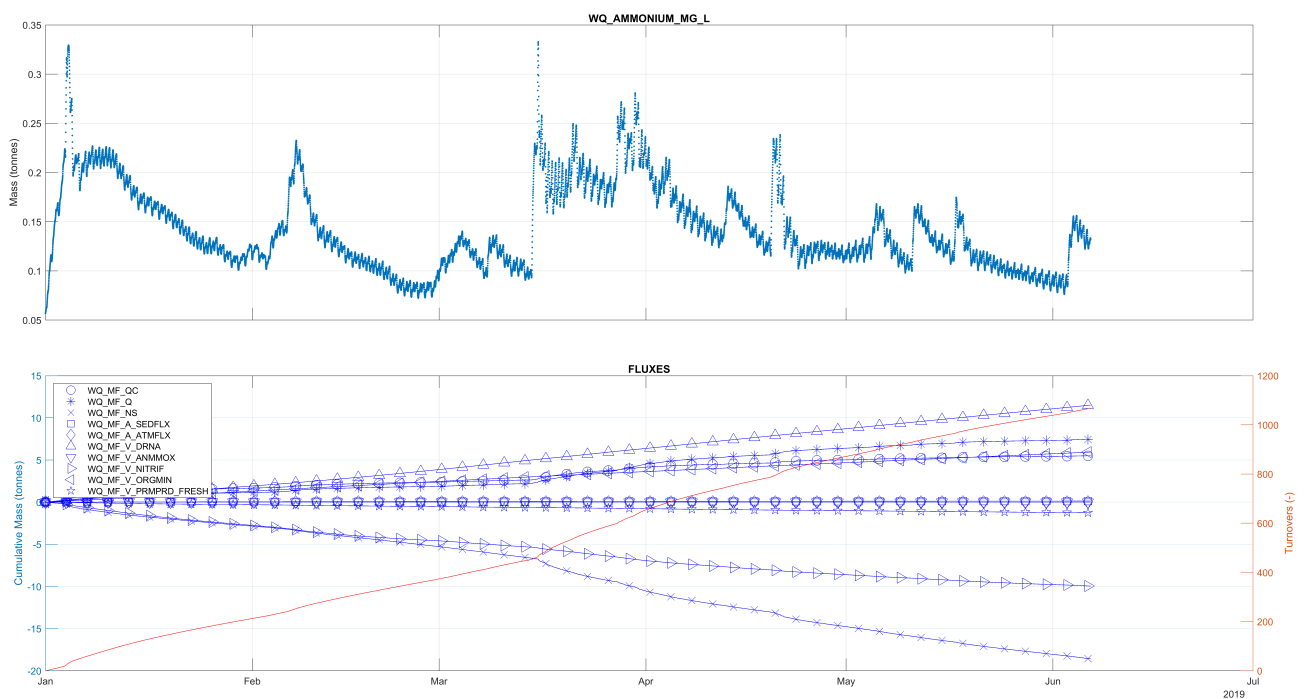


Figure 4.4: Mass balance output: Ammonium

Each mass balance output .csv file consists of columnar timeseries data, with column headers presented and described in the following tables:

- DO Simulation Class: Table 4.1
 - Dissolved oxygen
- Inorganics Simulation Class: Table 4.2
 - Dissolved oxygen
 - Silicate
 - Ammonium

- Nitrate
- FRP
- Phytoplankton
- Organics Simulation Class: Table 4.3
 - Dissolved oxygen
 - Silicate
 - Ammonium
 - Nitrate
 - FRP
 - DOC
 - POC
 - DON
 - PON
 - DOP
 - POP
 - RDOC
 - RDON
 - RDOP
 - RPOM
 - Phytoplankton

Acronyms within column headers include:

- V = Volumetric quantity
- A = Areal quantity
- MF = Mass flux
- FV = TUFLOW FV output or computed from same
- NS = Nodestring, encompassing WL, WLS and QN boundary types
- WQ = Water Quality output or computed from same
- Q = Q boundary type
- QC = QC or QC_POLY boundary types
- PCT = Percent
- pn = phytoplankton name

Table 4.1: Water Quality Mass Flux Headers - DO Simulation Class

Simulation Class	DO	
Dissolved Oxygen	<fvc_name>_MASSBALANCE_WQ DISS_OXYGEN_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous dissolved oxygen mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes O ₂
WQ_MF_QC	Accumulated dissolved oxygen mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes O ₂
WQ_MF_Q	Accumulated dissolved oxygen mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes O ₂
WQ_MF_NS	Accumulated dissolved oxygen mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes O ₂
WQ_MF_A_SED-FLX	Accumulated dissolved oxygen mass flux due to sediment consumption or production across the entire domain, summed to a single timeseries. Can be a positive or negative quantity.	tonnes O ₂
WQ_MF_A_ATM-FLX	Accumulated dissolved oxygen mass flux due to atmospheric exchange across the entire domain, summed to a single timeseries. Can be a positive or negative quantity.	tonnes O ₂

Table 4.1: Water Quality Mass Flux Headers - DO Simulation Class

Simulation Class	DO	
WQ_MF_TOTAL	Total of accumulated dissolved oxygen mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes O ₂
MF_WQ_MASS	Estimate of total dissolved oxygen mass computed from summing previous timestep dissolved oxygen mass (MF_WQ_MASS) and current timestep (not cumulative) dissolved oxygen mass fluxes. See Section Q.4 for details. Always a positive quantity.	tonnes O ₂
MF_PCT_ERROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units

Table 4.2: Water Quality Mass Flux Headers - Inorganics Simulation Class

Simulation Class	Inorganics	
Dissolved Oxygen	<fvc_name>_MASSBALANCE_WQ DISS_OXYGEN_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous dissolved oxygen mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes O ₂
WQ_MF_QC	Accumulated dissolved oxygen mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes O ₂
WQ_MF_Q	Accumulated dissolved oxygen mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes O ₂
WQ_MF_NS	Accumulated dissolved oxygen mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes O ₂
WQ_MF_A_SED-FLX	Accumulated dissolved oxygen mass flux due to sediment consumption or production across the entire domain, summed to a single timeseries. Can be a positive or negative quantity.	tonnes O ₂
WQ_MF_A_ATM-FLX	Accumulated dissolved oxygen mass flux due to atmospheric exchange across the entire domain, summed to a single timeseries. Can be a positive or negative quantity.	tonnes O ₂
WQ_MF_V_NITRIF	Accumulated dissolved oxygen mass flux due to consumption through nitrification across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes O ₂
WQ_MF_V_PRM-PRD_<PN>	Accumulated dissolved oxygen mass flux due to production through phytoplankton primary productivity across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a positive quantity.	tonnes O ₂

Table 4.2: Water Quality Mass Flux Headers - Inorganics Simulation Class

Simulation Class	Inorganics	
WQ_MF_V_RESPIR_<PN>	Accumulated dissolved oxygen mass flux due to consumption through phytoplankton respiration across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a negative quantity.	tonnes O ₂
WQ_MF_TOTAL	Total of accumulated dissolved oxygen mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes O ₂
MF_WQ_MASS	Estimate of total dissolved oxygen mass computed from summing previous timestep dissolved oxygen mass (MF_WQ_MASS) and current timestep (not cumulative) dissolved oxygen mass fluxes. See Section Q.4 for details. Always a positive quantity.	tonnes O ₂
MF_PCT_ERROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
Silicate	<fvc_name>_MASSBALANCE_WQ_SILICATE_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous silicate mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes Si
WQ_MF_QC	Accumulated silicate mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes Si
WQ_MF_Q	Accumulated silicate mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes Si
WQ_MF_NS	Accumulated silicate mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes Si
WQ_MF_A_SED-FLX	Accumulated silicate mass flux due to sediment consumption or production across the entire domain, summed to a single timeseries. Can be a positive or negative quantity.	tonnes Si
WQ_MF_V_PRM-PRD_<PN>	Accumulated silicate mass flux due to consumption through phytoplankton primary productivity across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group that uptakes silicate, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are silicate based phytoplankton groups. No column is included for phytoplankton groups that do not include silicate uptake. Always a negative quantity.	tonnes Si
WQ_MF_V_MORTAL_<PN>	Accumulated silicate mass flux due to production through phytoplankton mortality across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group that uptakes silicate, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are silicate based phytoplankton groups. No column is included for phytoplankton groups that do not include silicate uptake. Always a positive quantity.	tonnes Si

Table 4.2: Water Quality Mass Flux Headers - Inorganics Simulation Class

Simulation Class	Inorganics	
WQ_MF_V_EX-CRET_<PN>	Accumulated silicate mass flux due to production through phytoplankton excretion across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group that uptakes silicate, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are silicate based phytoplankton groups. No column is included for phytoplankton groups that do not include silicate uptake. Always a positive quantity.	tonnes Si
WQ_MF_TOTAL	Total of accumulated silicate mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes Si
MF_WQ_MASS	Estimate of total silicate mass computed from summing previous timestep silicate mass (MF_WQ_MASS) and current timestep (not cumulative) silicate mass fluxes. See Section Q.4 for details. Always a positive quantity.	tonnes Si
MF_PCT_ERROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
Ammonium	<fvc_name>_MASSBALANCE_WQ_AMMONIUM_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous ammonium mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes N
WQ_MF_QC	Accumulated ammonium mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_Q	Accumulated ammonium mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_NS	Accumulated ammonium mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_A_SED-FLX	Accumulated ammonium mass flux due to sediment consumption or production across the entire domain, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_A_ATM-FLX	Accumulated ammonium mass flux due to atmospheric exchange across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes N
WQ_MF_V_DRNA	Accumulated ammonium mass flux due to dissimilatory reduction of nitrate to ammonium across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes N
WQ_MF_V_AN-MMOX	Accumulated ammonium mass flux due to anaerobic oxidation of ammonium to nitrate across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes N
WQ_MF_V_NI-TRIF	Accumulated ammonium mass flux due to nitrification across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes N
WQ_MF_V_PRM-PRD_<PN>	Accumulated ammonium mass flux due to consumption through phytoplankton primary productivity across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a negative quantity.	tonnes N

Table 4.2: Water Quality Mass Flux Headers - Inorganics Simulation Class

Simulation Class	Inorganics	
WQ_MF_V_MORTAL_<PN>	Accumulated ammonium mass flux due to production through phytoplankton mortality across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a positive quantity.	tonnes N
WQ_MF_V_EXCRET_<PN>	Accumulated ammonium mass flux due to production through phytoplankton excretion across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a positive quantity.	tonnes N
WQ_MF_TOTAL	Total of accumulated ammonium mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes N
MF_WQ_MASS	Estimate of total ammonium mass computed from summing previous timestep ammonium mass (MF_WQ_MASS) and current timestep (not cumulative) ammonium mass fluxes. See Section 4.4 for details. Always a positive quantity.	tonnes N
MF_PCT_ERROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
Nitrate	<fvc_name>_MASSBALANCE_WQ_NITRATE_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous nitrate mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes N
WQ_MF_QC	Accumulated nitrate mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_Q	Accumulated nitrate mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_NS	Accumulated nitrate mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_A_SED-FLX	Accumulated nitrate mass flux due to sediment consumption or production across the entire domain, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_A_ATM-FLX	Accumulated nitrate mass flux due to atmospheric exchange across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes N
WQ_MF_V_DRNA	Accumulated nitrate mass flux due to dissimilatory reduction of nitrate to ammonium across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes N
WQ_MF_V_AN-MMOX	Accumulated nitrate mass flux due to anaerobic oxidation of ammonium to nitrate across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes N
WQ_MF_V_NI-TRIF	Accumulated nitrate mass flux due to nitrification across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes N
WQ_MF_V_DEN-TRF	Accumulated nitrate mass flux due to denitrification across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes N

Table 4.2: Water Quality Mass Flux Headers - Inorganics Simulation Class

Simulation Class	Inorganics	
WQ_MF_V_PRM-PRD_<PN>	Accumulated nitrate mass flux due to consumption through phytoplankton primary productivity across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a negative quantity.	tonnes N
WQ_MF_TOTAL	Total of accumulated nitrate mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes N
MF_WQ_MASS	Estimate of total nitrate mass computed from summing previous timestep nitrate mass (MF_WQ_MASS) and current timestep (not cumulative) nitrate mass fluxes. See Section Q.4 for details. Always a positive quantity.	tonnes N
MF_PCT_ER-ROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
FRP	<fvc_name>_MASSBALANCE_WQ_FRP_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous FRP (and adsorbed FRP, if simulated) mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes P
WQ_MF_QC	Accumulated FRP (and adsorbed FRP, if simulated) mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes P
WQ_MF_Q	Accumulated FRP (and adsorbed FRP, if simulated) mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes P
WQ_MF_NS	Accumulated FRP (and adsorbed FRP, if simulated) mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes P
WQ_MF_A_SED-FLX	Accumulated FRP mass flux due to sediment consumption or production across the entire domain, summed to a single timeseries. Can be a positive or negative quantity.	tonnes P
WQ_MF_A_ATM-FLX	Accumulated FRP (and adsorbed FRP, if simulated) mass flux due to atmospheric exchange across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes P
WQ_MF_V_ADS-DSP	Accumulated FRP adsorption. This output is not supported so is reported as zeros. Column only included if adsorbed FRP is simulated.	tonnes P
WQ_MF_V_SEDMTNf	If simulated, accumulated adsorbed FRP settling to sediments across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes P
WQ_MF_V_PRM-PRD_<PN>	Accumulated FRP mass flux due to consumption through phytoplankton primary productivity across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a negative quantity.	tonnes P

Table 4.2: Water Quality Mass Flux Headers - Inorganics Simulation Class

Simulation Class	Inorganics	
WQ_MF_V_MORTAL_<PN>	Accumulated FRP mass flux due to production through phytoplankton mortality across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a positive quantity.	tonnes P
WQ_MF_V_EXCRET_<PN>	Accumulated FRP mass flux due to production through phytoplankton excretion across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a positive quantity.	tonnes P
WQ_MF_TOTAL	Total of accumulated FRP (and adsorbed FRP, if simulated) mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes P
MF_WQ_MASS	Estimate of total FRP (and adsorbed FRP, if simulated) mass computed from summing previous timestep ammonium mass (MF_WQ_MASS) and current timestep (not cumulative) ammonium mass fluxes. See Section 4.4 for details. Always a positive quantity.	tonnes P
MF_PCT_ERROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
Phytoplankton TIME	<fvc_name>_MASSBALANCE_WQ_PHYTO_<PN>_CONC_MICG_L.csv ISODATE Time	Units
FV_WQ_MASS	Instantaneous phytoplankton group mass computed from TUFLOW FV state variables. Always a positive quantity.	kg Chla
WQ_MF_QC	Accumulated phytoplankton group mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	kg Chla
WQ_MF_Q	Accumulated phytoplankton mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	kg Chla
WQ_MF_NS	Accumulated phytoplankton mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	kg Chla
WQ_MF_V_PRMPRD	Accumulated phytoplankton mass flux due to primary productivity across the entire domain, summed to a single timeseries. Always a positive quantity.	kg Chla
WQ_MF_V_RESPIR	Accumulated phytoplankton mass flux due to respiration across the entire domain, summed to a single timeseries. Always a negative quantity.	kg Chla
WQ_MF_V_MORTAL	Accumulated phytoplankton mass flux due to mortality across the entire domain, summed to a single timeseries. Always a negative quantity.	kg Chla
WQ_MF_V_EXCRET	Accumulated phytoplankton mass flux due to excretion across the entire domain, summed to a single timeseries. Always a negative quantity.	kg Chla
WQ_MF_V_SEDMTN	Accumulated phytoplankton mass flux due to settling to sediments across the entire domain, summed to a single timeseries. Always a negative quantity.	kg Chla
WQ_MF_TOTAL	Total of accumulated phytoplankton mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	kg Chla

Table 4.2: Water Quality Mass Flux Headers - Inorganics Simulation Class

Simulation Class	Inorganics	
MF_WQ_MASS	Estimate of total phytoplankton mass computed from summing previous timestep phytoplankton mass (MF_WQ_MASS) and current timestep (not cumulative) phytoplankton mass fluxes. See Section Q.4 for details. Always a positive quantity.	kg Chla
MF_PCT_ERROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units

Table 4.3: Water Quality Mass Flux Headers - Organics Simulation Class

Simulation Class	Organics	
Dissolved Oxygen	<fvc_name>_MASSBALANCE_WQ DISS_OXYGEN_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous dissolved oxygen mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes O ₂
WQ_MF_QC	Accumulated dissolved oxygen mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes O ₂
WQ_MF_Q	Accumulated dissolved oxygen mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes O ₂
WQ_MF_NS	Accumulated dissolved oxygen mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes O ₂
WQ_MF_A_SED-FLX	Accumulated dissolved oxygen mass flux due to sediment consumption or production across the entire domain, summed to a single timeseries. Can be a positive or negative quantity.	tonnes O ₂
WQ_MF_A_ATM-FLX	Accumulated dissolved oxygen mass flux due to atmospheric exchange across the entire domain, summed to a single timeseries. Can be a positive or negative quantity.	tonnes O ₂
WQ_MF_V_NITRIF	Accumulated dissolved oxygen mass flux due to consumption through nitrification across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes O ₂
WQ_MF_V_AERMIN	Accumulated dissolved oxygen mass flux due to consumption through aerobic mineralisation of organic matter across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes O ₂
WQ_MF_V_PRRD-<PN>	Accumulated dissolved oxygen mass flux due to production through phytoplankton primary productivity across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a positive quantity.	tonnes O ₂

Table 4.3: Water Quality Mass Flux Headers - Organics Simulation Class

Simulation Class	Organics	
WQ_MF_V_RESPIR_<PN>	Accumulated dissolved oxygen mass flux due to consumption through phytoplankton respiration across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a negative quantity.	tonnes O ₂
WQ_MF_TOTAL	Total of accumulated dissolved oxygen mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes O ₂
MF_WQ_MASS	Estimate of total dissolved oxygen mass computed from summing previous timestep dissolved oxygen mass (MF_WQ_MASS) and current timestep (not cumulative) dissolved oxygen mass fluxes. See Section Q.4 for details. Always a positive quantity.	tonnes O ₂
MF_PCT_ERROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
Silicate	<fvc_name>_MASSBALANCE_WQ_SILICATE_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous silicate mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes Si
WQ_MF_QC	Accumulated silicate mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes Si
WQ_MF_Q	Accumulated silicate mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes Si
WQ_MF_NS	Accumulated silicate mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes Si
WQ_MF_A_SED-FLX	Accumulated silicate mass flux due to sediment consumption or production across the entire domain, summed to a single timeseries. Can be a positive or negative quantity.	tonnes Si
WQ_MF_V_PRD-PRD_<PN>	Accumulated silicate mass flux due to consumption through phytoplankton primary productivity across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group that uptakes silicate, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are silicate based phytoplankton groups. No column is included for phytoplankton groups that do not include silicate uptake. Always a negative quantity.	tonnes Si
WQ_MF_V_MORTAL_<PN>	Accumulated silicate mass flux due to production through phytoplankton mortality across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group that uptakes silicate, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are silicate based phytoplankton groups. No column is included for phytoplankton groups that do not include silicate uptake. Always a positive quantity.	tonnes Si

Table 4.3: Water Quality Mass Flux Headers - Organics Simulation Class

Simulation Class	Organics	
WQ_MF_V_EX-CRET_<PN>	Accumulated silicate mass flux due to production through phytoplankton excretion across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group that uptakes silicate, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are silicate based phytoplankton groups. No column is included for phytoplankton groups that do not include silicate uptake. Always a positive quantity.	tonnes Si
WQ_MF_TOTAL	Total of accumulated silicate mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes Si
MF_WQ_MASS	Estimate of total silicate mass computed from summing previous timestep silicate mass (MF_WQ_MASS) and current timestep (not cumulative) silicate mass fluxes. See Section Q.4 for details. Always a positive quantity.	tonnes Si
MF_PCT_ERROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
Ammonium	<fvc_name>_MASSBALANCE_WQ_AMMONIUM_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous ammonium mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes N
WQ_MF_QC	Accumulated ammonium mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_Q	Accumulated ammonium mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_NS	Accumulated ammonium mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_A_SED-FLX	Accumulated ammonium mass flux due to sediment consumption or production across the entire domain, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_A_ATM-FLX	Accumulated ammonium mass flux due to atmospheric exchange across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes N
WQ_MF_V_DRNA	Accumulated ammonium mass flux due to dissimilatory reduction of nitrate to ammonium across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes N
WQ_MF_V_AN-MMOX	Accumulated ammonium mass flux due to anaerobic oxidation of ammonium to nitrate across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes N
WQ_MF_V_NI-TRIF	Accumulated ammonium mass flux due to nitrification across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes N
WQ_MF_V_ORGMIN	Accumulated ammonium mass flux due to mineralisation of labile dissolved organic nitrogen across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes N
WQ_MF_V_PHO-TOL	Accumulated ammonium mass flux due to photolysis of refractory organic nitrogen (if simulated) across the entire domain (if photolysis is switched on), summed to a single timeseries. Always a positive quantity.	tonnes N

Table 4.3: Water Quality Mass Flux Headers - Organics Simulation Class

Simulation Class	Organics	
WQ_MF_V_PRM-PRD_<PN>	Accumulated ammonium mass flux due to consumption through phytoplankton primary productivity across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a negative quantity.	tonnes N
WQ_MF_TOTAL	Total of accumulated ammonium mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes N
MF_WQ_MASS	Estimate of total ammonium mass computed from summing previous timestep ammonium mass (MF_WQ_MASS) and current timestep (not cumulative) ammonium mass fluxes. See Section Q.4 for details. Always a positive quantity.	tonnes N
MF_PCT_ER-ROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
Nitrate	<fvc_name>_MASSBALANCE_WQ_NITRATE_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous nitrate mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes N
WQ_MF_QC	Accumulated nitrate mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_Q	Accumulated nitrate mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_NS	Accumulated nitrate mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_A_SED-FLX	Accumulated nitrate mass flux due to sediment consumption or production across the entire domain, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_A_ATM-FLX	Accumulated nitrate mass flux due to atmospheric exchange across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes N
WQ_MF_V_DRNA	Accumulated nitrate mass flux due to dissimilatory reduction of nitrate to ammonium across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes N
WQ_MF_V_AN-MMOX	Accumulated nitrate mass flux due to anaerobic oxidation of ammonium to nitrate across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes N
WQ_MF_V_NI-TRIF	Accumulated nitrate mass flux due to nitrification across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes N
WQ_MF_V_DEN-TRF	Accumulated nitrate mass flux due to denitrification across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes N
WQ_MF_V_NO3MIN	Accumulated nitrogen mass flux due to mineralisation of labile dissolved organic nitrogen (using nitrate as an oxygen source) across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes N

Table 4.3: Water Quality Mass Flux Headers - Organics Simulation Class

Simulation Class	Organics	
**WQ_MF_V_PRM-PRD_<PN>	Accumulated nitrate mass flux due to consumption through phytoplankton primary productivity across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a negative quantity.	tonnes N
WQ_MF_TOTAL	Total of accumulated nitrate mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes N
MF_WQ_MASS	Estimate of total nitrate mass computed from summing previous timestep nitrate mass (MF_WQ_MASS) and current timestep (not cumulative) nitrate mass fluxes. See Section Q.4 for details. Always a positive quantity.	tonnes N
MF_PCT_ER-ROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
FRP	<fvc_name>_MASSBALANCE_WQ_FRP_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous FRP (and adsorbed FRP, if simulated) mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes P
WQ_MF_QC	Accumulated FRP (and adsorbed FRP, if simulated) mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes P
WQ_MF_Q	Accumulated FRP (and adsorbed FRP, if simulated) mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes P
WQ_MF_NS	Accumulated FRP (and adsorbed FRP, if simulated) mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes P
WQ_MF_A_SED-FLX	Accumulated FRP mass flux due to sediment consumption or production across the entire domain, summed to a single timeseries. Can be a positive or negative quantity.	tonnes P
WQ_MF_A_ATM-FLX	Accumulated FRP (and adsorbed FRP, if simulated) mass flux due to atmospheric exchange across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes P
WQ_MF_V_ADS-DSP	Accumulated FRP adsorption. This output is not supported so is reported as zeros. Column only included if adsorbed FRP is simulated.	tonnes P
WQ_MF_V_SEDMTNf	If simulated, accumulated adsorbed FRP settling to sediments across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes P
WQ_MF_V_ORGMIN	Accumulated FRP mass flux due to mineralisation of labile dissolved organic phosphorus across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes P
WQ_MF_V_PHO-TOL	Accumulated FRP mass flux due to photolysis of refractory organic phosphorus (if simulated) across the entire domain (if photolysis is switched on), summed to a single timeseries. Always a positive quantity.	tonnes P

Table 4.3: Water Quality Mass Flux Headers - Organics Simulation Class

Simulation Class	Organics	
WQ_MF_V_PRM-PRD_<PN>	Accumulated FRP mass flux due to consumption through phytoplankton primary productivity across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a negative quantity.	tonnes P
WQ_MF_TOTAL	Total of accumulated FRP (and adsorbed FRP, if simulated) mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes P
MF_WQ_MASS	Estimate of total FRP (and adsorbed FRP, if simulated) mass computed from summing previous timestep ammonium mass (MF_WQ_MASS) and current timestep (not cumulative) ammonium mass fluxes. See Section Q.4 for details. Always a positive quantity.	tonnes P
MF_PCT_ER-ROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
Labile dissolved organic carbon	<fvc_name>_MASSBALANCE_WQ_DOC_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous labile dissolved organic carbon mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes C
WQ_MF_QC	Accumulated labile dissolved organic carbon mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes C
WQ_MF_Q	Accumulated labile dissolved organic carbon mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes C
WQ_MF_NS	Accumulated labile dissolved organic carbon mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes C
WQ_MF_A_SED-FLX	Accumulated labile dissolved organic carbon mass flux due to sediment consumption or production across the entire domain, summed to a single timeseries. Can be a positive or negative quantity.	tonnes C
WQ_MF_V_HY-DLSS	Accumulated labile dissolved organic carbon mass flux due to hydrolysis of labile particulate organic carbon across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes C
WQ_MF_V_ORGMINA	Accumulated labile dissolved organic carbon mass flux due to mineralisation of labile dissolved organic carbon across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes C
WQ_MF_V_ACTIVN	Accumulated labile dissolved organic carbon mass flux due to activation of refractory dissolved organic carbon (if simulated) across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes C
WQ_MF_V_PHO-TOL	Accumulated labile dissolved organic carbon mass flux due to photolysis of refractory organic carbon (if simulated) across the entire domain (if photolysis is switched on), summed to a single timeseries. Always a positive quantity.	tonnes C

Table 4.3: Water Quality Mass Flux Headers - Organics Simulation Class

Simulation Class	Organics	
WQ_MF_V_EX-CRET_<PN>	Accumulated labile dissolved organic carbon mass flux due to production through phytoplankton excretion across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a positive quantity.	tonnes C
WQ_MF_TOTAL	Total of accumulated labile dissolved organic carbon mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes C
MF_WQ_MASS	Estimate of total labile dissolved organic carbon mass computed from summing previous timestep labile dissolved organic carbon mass (MF_WQ_MASS) and current timestep (not cumulative) labile dissolved organic carbon mass fluxes. See Section Q.4 for details. Always a positive quantity.	tonnes C
MF_PCT_ER-ROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
Labile particulate organic carbon	<fvc_name>_MASSBALANCE_WQ_POC_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous labile particulate organic carbon mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes C
WQ_MF_QC	Accumulated labile particulate organic carbon mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes C
WQ_MF_Q	Accumulated labile particulate organic carbon mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes C
WQ_MF_NS	Accumulated labile particulate organic carbon mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes C
WQ_MF_V_HY-DLSS	Accumulated labile particulate organic carbon mass flux due to hydrolysis of labile particulate organic carbon across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes C
WQ_MF_V_SEDMTN	Accumulated labile particulate organic carbon mass settling to sediments across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes C
WQ_MF_V_BRKDOWN	Accumulated labile particulate organic carbon mass flux due to the breakdown of refractory particulate organic matter (if simulated) across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes C
WQ_MF_V_MORTAL_<PN>	Accumulated labile particulate organic carbon mass flux due to production through phytoplankton mortality across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a positive quantity.	tonnes C
WQ_MF_TOTAL	Total of accumulated labile particulate organic carbon mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes C

Table 4.3: Water Quality Mass Flux Headers - Organics Simulation Class

Simulation Class	Organics	
MF_WQ_MASS	Estimate of total labile particulate organic carbon mass computed from summing previous timestep labile particulate organic carbon mass (MF_WQ_MASS) and current timestep (not cumulative) labile particulate organic carbon mass fluxes. See Section Q.4 for details. Always a positive quantity.	tonnes C
MF_PCT_ERROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
Labile dissolved organic nitrogen	<fvc_name>_MASSBALANCE_WQ_DON_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous labile dissolved organic nitrogen mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes N
WQ_MF_QC	Accumulated labile dissolved organic nitrogen mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_Q	Accumulated labile dissolved organic nitrogen mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_NS	Accumulated labile dissolved organic nitrogen mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_A_SED-FLX	Accumulated labile dissolved organic nitrogen mass flux due to sediment consumption or production across the entire domain, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_V_HY-DLSS	Accumulated labile dissolved organic nitrogen mass flux due to hydrolysis of labile particulate organic nitrogen across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes N
WQ_MF_V_ORGMIN	Accumulated labile dissolved organic nitrogen mass flux due to mineralisation of labile dissolved organic nitrogen across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes N
WQ_MF_V_ACTIVN	Accumulated labile dissolved organic nitrogen mass flux due to activation of refractory dissolved organic nitrogen (if simulated) across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes N
WQ_MF_V_PHOTOL	Accumulated labile dissolved organic nitrogen mass flux due to photolysis of refractory organic nitrogen (if simulated) across the entire domain (if photolysis is switched on), summed to a single timeseries. Always a positive quantity.	tonnes N
WQ_MF_V_EXCRET_<PN>	Accumulated labile dissolved organic nitrogen mass flux due to production through phytoplankton excretion across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a positive quantity.	tonnes N
WQ_MF_TOTAL	Total of accumulated labile dissolved organic nitrogen mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes N

Table 4.3: Water Quality Mass Flux Headers - Organics Simulation Class

Simulation Class	Organics	
MF_WQ_MASS	Estimate of total labile dissolved organic nitrogen mass computed from summing previous timestep labile dissolved organic nitrogen mass (MF_WQ_MASS) and current timestep (not cumulative) labile dissolved organic nitrogen mass fluxes. See Section Q.4 for details. Always a positive quantity.	tonnes N
MF_PCT_ERROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
Labile particulate organic nitrogen	<fvc_name>_MASSBALANCE_WQ_PON_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous labile particulate organic nitrogen mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes N
WQ_MF_QC	Accumulated labile particulate organic nitrogen mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_Q	Accumulated labile particulate organic nitrogen mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_NS	Accumulated labile particulate organic nitrogen mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_V_HYDLSS	Accumulated labile particulate organic nitrogen mass flux due to hydrolysis of labile particulate organic nitrogen across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes N
WQ_MF_V_SEDMTN	Accumulated labile particulate organic nitrogen mass settling to sediments across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes N
WQ_MF_V_BRKDOWN	Accumulated labile particulate organic nitrogen mass flux due to the breakdown of refractory particulate organic matter (if simulated) across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes N
WQ_MF_V_MORTAL_<PN>	Accumulated labile particulate organic nitrogen mass flux due to production through phytoplankton mortality across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a positive quantity.	tonnes N
WQ_MF_TOTAL	Total of accumulated labile particulate organic nitrogen mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes N
MF_WQ_MASS	Estimate of total labile particulate organic nitrogen mass computed from summing previous timestep labile particulate organic nitrogen mass (MF_WQ_MASS) and current timestep (not cumulative) labile particulate organic nitrogen mass fluxes. See Section Q.4 for details. Always a positive quantity.	tonnes N
MF_PCT_ERROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	

Table 4.3: Water Quality Mass Flux Headers - Organics Simulation Class

Simulation Class	Organics	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
Labile dissolved organic phosphorus	<fvc_name>_MASSBALANCE_WQ_DOP_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous labile dissolved organic phosphorus mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes P
WQ_MF_QC	Accumulated labile dissolved organic phosphorus mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes P
WQ_MF_Q	Accumulated labile dissolved organic phosphorus mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes P
WQ_MF_NS	Accumulated labile dissolved organic phosphorus mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes P
WQ_MF_A_SED-FLX	Accumulated labile dissolved organic phosphorus mass flux due to sediment consumption or production across the entire domain, summed to a single timeseries. Can be a positive or negative quantity.	tonnes P
WQ_MF_V_HY-DLSS	Accumulated labile dissolved organic phosphorus mass flux due to hydrolysis of labile particulate organic phosphorus across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes P
WQ_MF_V_ORGMIN	Accumulated labile dissolved organic phosphorus mass flux due to mineralisation of labile dissolved organic phosphorus across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes P
WQ_MF_V_ACTIVN	Accumulated labile dissolved organic phosphorus mass flux due to activation of refractory dissolved organic phosphorus (if simulated) across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes P
WQ_MF_V_PHOTOL	Accumulated labile dissolved organic phosphorus mass flux due to photolysis of refractory organic phosphorus (if simulated) across the entire domain (if photolysis is switched on), summed to a single timeseries. Always a positive quantity.	tonnes P
WQ_MF_V_EXCRET_<PN>	Accumulated labile dissolved organic phosphorus mass flux due to production through phytoplankton excretion across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a positive quantity.	tonnes P
WQ_MF_TOTAL	Total of accumulated labile dissolved organic phosphorus mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes P
MF_WQ_MASS	Estimate of total labile dissolved organic phosphorus mass computed from summing previous timestep labile dissolved organic phosphorus mass (MF_WQ_MASS) and current timestep (not cumulative) labile dissolved organic phosphorus mass fluxes. See Section 4.4 for details. Always a positive quantity.	tonnes P
MF_PCT_ERROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	

Table 4.3: Water Quality Mass Flux Headers - Organics Simulation Class

Simulation Class	Organics	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
Labile particulate organic phosphorus	<fvc_name>_MASSBALANCE_WQ_POP_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous labile particulate organic phosphorus mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes P
WQ_MF_QC	Accumulated labile particulate organic phosphorus mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes P
WQ_MF_Q	Accumulated labile particulate organic phosphorus mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes P
WQ_MF_NS	Accumulated labile particulate organic phosphorus mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes P
WQ_MF_V_HY-DLSS	Accumulated labile particulate organic phosphorus mass flux due to hydrolysis of labile particulate organic phosphorus across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes P
WQ_MF_V_SEDMTN	Accumulated labile particulate organic phosphorus mass settling to sediments across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes P
WQ_MF_V_BRKDOWN	Accumulated labile particulate organic phosphorus mass flux due to the breakdown of refractory particulate organic matter (if simulated) across the entire domain, summed to a single timeseries. Always a positive quantity.	tonnes P
WQ_MF_V_MORTAL<PN>	Accumulated labile particulate organic phosphorus mass flux due to production through phytoplankton mortality across the entire domain, summed to a single timeseries. The accumulated mass flux is reported separately for each phytoplankton group, so this field will be repeated (with a different <PN> inserted in each column header) for as many columns as there are phytoplankton groups. Always a positive quantity.	tonnes P
WQ_MF_TOTAL	Total of accumulated labile particulate organic phosphorus mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes P
MF_WQ_MASS	Estimate of total labile particulate organic phosphorus mass computed from summing previous timestep labile particulate organic phosphorus mass (MF_WQ_MASS) and current timestep (not cumulative) labile particulate organic phosphorus mass fluxes. See Section Q.4 for details. Always a positive quantity.	tonnes P
MF_PCT_ERROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
Refractory dissolved organic carbon	<fvc_name>_MASSBALANCE_WQ_RDOC_MG_L.csv	Units
TIME	ISODATE Time	

Table 4.3: Water Quality Mass Flux Headers - Organics Simulation Class

Simulation Class	Organics	
FV_WQ_MASS	Instantaneous refractory dissolved organic carbon mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes C
WQ_MF_QC	Accumulated refractory dissolved organic carbon mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes C
WQ_MF_Q	Accumulated refractory dissolved organic carbon mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes C
WQ_MF_NS	Accumulated refractory dissolved organic carbon mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes C
WQ_MF_V_ACTIVN	Accumulated refractory dissolved organic carbon mass flux due to activation of refractory dissolved organic carbon (if simulated) across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes C
WQ_MF_V_PHOTOL	Accumulated refractory dissolved organic carbon mass flux due to photolysis of refractory organic carbon (if simulated) across the entire domain (if photolysis is switched on), summed to a single timeseries. Always a negative quantity.	tonnes C
WQ_MF_TOTAL	Total of accumulated refractory dissolved organic carbon mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes C
MF_WQ_MASS	Estimate of total refractory dissolved organic carbon mass computed from summing previous timestep refractory dissolved organic carbon mass (MF_WQ_MASS) and current timestep (not cumulative) refractory dissolved organic carbon mass fluxes. See Section 4.4 for details. Always a positive quantity.	tonnes C
MF_PCT_ERROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
Refractory dissolved organic nitrogen	<fvc_name>_MASSBALANCE_WQ_RDON_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous refractory dissolved organic nitrogen mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes N
WQ_MF_QC	Accumulated refractory dissolved organic nitrogen mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_Q	Accumulated refractory dissolved organic nitrogen mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_NS	Accumulated refractory dissolved organic nitrogen mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes N
WQ_MF_V_ACTIVN	Accumulated refractory dissolved organic nitrogen mass flux due to activation of refractory dissolved organic nitrogen (if simulated) across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes N

Table 4.3: Water Quality Mass Flux Headers - Organics Simulation Class

Simulation Class	Organics	
WQ_MF_V_PHOTOL	Accumulated refractory dissolved organic nitrogen mass flux due to photolysis of refractory organic nitrogen (if simulated) across the entire domain (if photolysis is switched on), summed to a single timeseries. Always a negative quantity.	tonnes N
WQ_MF_TOTAL	Total of accumulated refractory dissolved organic nitrogen mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes N
MF_WQ_MASS	Estimate of total refractory dissolved organic nitrogen mass computed from summing previous timestep refractory dissolved organic nitrogen mass (MF_WQ_MASS) and current timestep (not cumulative) refractory dissolved organic nitrogen mass fluxes. See Section Q.4 for details. Always a positive quantity.	tonnes N
MF_PCT_ERROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
Refractory dissolved organic phosphorus TIME	<fvc_name>_MASSBALANCE_WQ_RDOP_MG_L.csv ISODATE Time	Units
FV_WQ_MASS	Instantaneous refractory dissolved organic phosphorus mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes P
WQ_MF_QC	Accumulated refractory dissolved organic phosphorus mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes P
WQ_MF_Q	Accumulated refractory dissolved organic phosphorus mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes P
WQ_MF_NS	Accumulated refractory dissolved organic phosphorus mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes P
WQ_MF_V_ACTIVATION	Accumulated refractory dissolved organic phosphorus mass flux due to activation of refractory dissolved organic phosphorus (if simulated) across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes P
WQ_MF_V_PHOTOL	Accumulated refractory dissolved organic phosphorus mass flux due to photolysis of refractory organic phosphorus (if simulated) across the entire domain (if photolysis is switched on), summed to a single timeseries. Always a negative quantity.	tonnes P
WQ_MF_TOTAL	Total of accumulated refractory dissolved organic phosphorus mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes P
MF_WQ_MASS	Estimate of total refractory dissolved organic phosphorus mass computed from summing previous timestep refractory dissolved organic phosphorus mass (MF_WQ_MASS) and current timestep (not cumulative) refractory dissolved organic phosphorus mass fluxes. See Section Q.4 for details. Always a positive quantity.	tonnes P
MF_PCT_ERROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units

Table 4.3: Water Quality Mass Flux Headers - Organics Simulation Class

Simulation Class	Organics	
Refractory particulate organic matter	<fvc_name>_MASSBALANCE_WQ_RPOM_MG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous refractory particulate organic matter mass computed from TUFLOW FV state variables. Always a positive quantity.	tonnes C
WQ_MF_QC	Accumulated refractory particulate organic matter mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes C
WQ_MF_Q	Accumulated refractory particulate organic matter mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes C
WQ_MF_NS	Accumulated refractory particulate organic matter mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	tonnes C
WQ_MF_V_BRKDOWN	Accumulated refractory particulate organic matter mass flux due to breakdown of refractory particulate organic matter (if simulated) across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes C
WQ_MF_V_SEDMTN	Accumulated refractory particulate organic matter mass settling to sediments across the entire domain, summed to a single timeseries. Always a negative quantity.	tonnes C
WQ_MF_TOTAL	Total of accumulated refractory particulate organic matter mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	tonnes C
MF_WQ_MASS	Estimate of total refractory particulate organic matter mass computed from summing previous timestep refractory particulate organic matter mass (MF_WQ_MASS) and current timestep (not cumulative) refractory particulate organic matter mass fluxes. See Section Q.4 for details. Always a positive quantity.	tonnes C
MF_PCT_ERROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units
Phytoplankton	<fvc_name>_MASSBALANCE_WQ_PHYTO_<PN>_CONC_MICG_L.csv	Units
TIME	ISODATE Time	
FV_WQ_MASS	Instantaneous phytoplankton group mass computed from TUFLOW FV state variables. Always a positive quantity.	kg Chla
WQ_MF_QC	Accumulated phytoplankton group mass fluxes across all QC and QC_POLY boundaries, summed to a single timeseries. Can be a positive or negative quantity.	kg Chla
WQ_MF_Q	Accumulated phytoplankton mass fluxes across all Q boundaries, summed to a single timeseries. Can be a positive or negative quantity.	kg Chla
WQ_MF_NS	Accumulated phytoplankton mass fluxes across all WL, WLS and QN boundaries, summed to a single timeseries. Can be a positive or negative quantity.	kg Chla
WQ_MF_V_PRM-PRD	Accumulated phytoplankton mass flux due to primary productivity across the entire domain, summed to a single timeseries. Always a positive quantity.	kg Chla
WQ_MF_V_RESPIR	Accumulated phytoplankton mass flux due to respiration across the entire domain, summed to a single timeseries. Always a negative quantity.	kg Chla

Table 4.3: Water Quality Mass Flux Headers - Organics Simulation Class

Simulation Class	Organics	
WQ_MF_V_MORTAL	Accumulated phytoplankton mass flux due to mortality across the entire domain, summed to a single timeseries. Always a negative quantity.	kg Chla
WQ_MF_V_EXCRET	Accumulated phytoplankton mass flux due to excretion across the entire domain, summed to a single timeseries. Always a negative quantity.	kg Chla
WQ_MF_V_SEDMTN	Accumulated phytoplankton mass flux due to settling to sediments across the entire domain, summed to a single timeseries. Always a negative quantity.	kg Chla
WQ_MF_TOTAL	Total of accumulated phytoplankton mass fluxes, with individual signs preserved. Can be a positive or negative quantity.	kg Chla
MF_WQ_MASS	Estimate of total phytoplankton mass computed from summing previous timestep phytoplankton mass (MF_WQ_MASS) and current timestep (not cumulative) phytoplankton mass fluxes. See Section Q.4 for details. Always a positive quantity.	kg Chla
MF_PCT_ERROR	The percentage difference between FV_WQ_MASS and MF_WQ_MASS . Can be a positive or negative quantity.	
MF_TURNOVERS	See explanatory text above and link to TUFLOW FV documentation (see Section 4.9.2). Always a positive quantity.	No units

4.9.3 Units

All output units are as set by the user (i.e. either the mg/L or mmol/m³ systems, noting that the latter is not supported by the mass balance outputs).

In binary outputs (i.e. NetCDF and DatV outputs) quantities are reported simply in the simulated units. The names of variables in these binary files will also denote the units of reporting. For example, dissolved oxygen concentrations reported in a three dimensional NetCDF file that was generated by a mg/L water quality simulation will:

- Be in units of mg/L. A reported value of “6.5” will be 6.5 mg/L
- Have the variable name `WQ_DISS_OXYGEN_MG_L`

In text based outputs (i.e. mass, flux and points outputs), units are reported in column headers. For consistency, SI units of kg, m³ and seconds are used to report in the mg/L system. In the mmol system, reporting units are moles, m³ and seconds. In both cases, these units may also deploy engineering notation (e.g. “x10³” or “x10⁶”) so that text field outputs are manageable. In these cases, the reported numbers in the columns have been multiplied by the noted magnitude in each header before being written to file. For example, a unit header of “x10³ kg” that subsequently reports a value of “4,000”, indicates that the simulated quantity was actually “4” kg - the simulated quantity has been multiplied by 10³ before being reported. Some specific examples of header notated units, and their simplifications include:

- mg/L system:
 - “x 10³ kg m⁻³” is mg/L
 - “x 10⁶ kg Chla m⁻³” is μ g/L
 - “x 10³ kg” is grams
 - “x 10⁶ kg” is milligrams
 - “x 10³ kg s⁻¹” is grams per second
- mmol/m³ system:
 - “x 10³ mol m⁻³” is mmol/m³
 - “x 10³ mol” is mmol
 - “x 10³ mol s⁻¹” is millimoles per second

Another way of thinking about this conversion is that if a unit is reported as “x 10^z units”, then the reported quantity needs to be divided by 10^z to recover the original quantity in “units”.

For diagnostic variables, the outputting of “points” (which are depth averaged), “mass” and “flux” files is rarely meaningful and should be avoided. No support for units of these output types is therefore provided. Binary files of these

outputs are meaningful (they are used in the mass balance analysis for example) so have the units of each diagnostic denoted in its name (e.g. “WQ_DIAG_FRP_ADS_SEDMTN_FLUX_MG_M2_D” is in $\text{mg}/\text{m}^2/\text{day}$).



A Commands

A.1 Overview

All WQ Module commands and descriptions are listed below ([FVWQ Commands](#)). For an explanation of command and parameter colour coding and notation, see [Commands](#) and [Parameters](#).

Commands in this appendix are documented in two types of entries:

1. **Implementation entries** appear as a command with an operator and parameters or input options (separated by |). For example, `Alive Min Max == [PTHa]pthmin, [PTHa]pthmax or Inorganic Phosphorus Model == FRPhs | FRPhsAds`

These document a specific form of a command and comprise the following components:

- Command heading: `command == parameter(s) or input option(s)`
- A summary block with the following information where applicable:
 - **Status:** whether the command is required, optional, conditional or legacy, along with a reason if applicable.
 - **Model Construction:** links to the construction sections in which the command is typically used.
 - **Required Dependent Command(s):** other commands that must be used alongside this command.
- Description: A paragraph describing what the command does, where it is used, and any important notes.
- Parameter subsections: For each parameter accepted by the command, a dedicated subsection follows. Where a command takes only a fixed set of options (such as `ON` or `OFF`), rather than numeric parameters, no parameter subsections follow the description.

The subsection heading shows the parameter symbol and its plain text name. A summary block provides:

- **Default:** the default value applied when the command is not specified. Where both unit systems are supported, defaults are shown as outlined above. `NA` indicates the parameter has no default and must be explicitly set.
- **Units:** the units for the parameter value. Where both unit systems are supported, units, range and default for both systems are listed in a table. See [Unit Systems](#) for more information on the unit systems.
- **Range:** an indicative range for the parameter value (see [Tip 1](#)). Where both unit systems are supported, range is shown as outlined above.
- **Science:** links to the science sections where the governing equations and background are described.

A description paragraph follows the summary block, providing context and guidance on how to set the parameter.

2. **Navigation entries** appear as a command heading with no operator (`==`) or parameters and therefore no parameter subsections. For example, `Adsorption`.

These are used where a command has multiple implementation variants, each with its own parameter set. The navigation entry identifies the command and directs users to the specific implementation entries that immediately follow. Not all commands have multiple implementation variants, so not all commands have navigation entries.

Note that all navigation entries specify 'Navigation row for this command' as some commands are not navigation entries but do not have any parameters (e.g. `End Material`).

Tip 1

Where parameter ranges are provided, these are not to be taken as fixed, but as indicative only. Some environmental settings may require parameterisation outside the ranges specified in this manual.

A.2 FVWQ Commands

Adsorption

Navigation row for this command. Argument syntax depends on the selected implementation. Refer to the implementation specific sections immediately below.

Adsorption == Linear, K_{ads-L}^{FRP}

Model Construction: Section 4.7.3.4.2

Used in an inorganic phosphorus constituent model block to set the paramters for the linear FRP adsorption model.

For further information on the linear adsorption model, refer to Section F.4.1.

K_{ads-L}^{FRP} - Linear FRP Sorption Partitioning Coefficient

Default: 0.01

Units: L/mg

Range: (0.01, 0.3)

Science: Section F.4

The coefficient that determines the partitioning of FRP between free and adsorbed states. Can be estimated by dividing adsorbed FRP by free FRP and the concentration of suspended sediment, if these three quantities are known

Adsorption == Quadratic, K_{ads-Q}^{FRP} , Q_{max}^{FRP}

Model Construction: Section 4.7.3.4.2

Used in a constituent model block to set the paramters for the quadratic FRP adsorption model.

For further information on the quadratic adsorption model, refer to Section F.4.2.

K_{ads-Q}^{FRP} - Quadratic FRP Sorption Partitioning Coefficient

Default: 0.7

Units: L/mg

Range: (0.6, 0.8)

Science: Section F.4

The ratio of adsorption and desorption rate coefficients for phosphorus

Q_{max}^{FRP} - Maximum Adsorption Capacity of Phosphorus

Default: 0.0051

Units: mg FRP-P/mg TSS

Range: (0.005, 0.006)

Science: Section F.4

The maximum mass of P that can be adsorbed onto ambient suspended sediment, per unit mass of suspended sediment

Alive Min Max == $[PTH_a]_{min}^{pth}$, $[PTH_a]_{max}^{pth}$

Model Construction: Section 4.6.3.2.1

Used in an (optional) pathogens constituent model block to set minimum and maximum alive (free) pathogen concentrations.

$[PTH_a]_{min}^{pth}$ - Minimum Alive Pathogen Concentration

Default: NA

Units: CFU/100mL

Range: (0, 0)

Science: Appendix N

The minimum allowable alive (free) pathogen concentration. If the WQ Module detects a concentration less than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues. A value other than zero for this parameter would be unusual

$[PTH_a]_{max}^{pth}$ - Maximum Alive Pathogen Concentration

Default: NA

Units: CFU/100mL

Range: (0, 1 e 12)

Science: Appendix N

The maximum allowable alive (free) pathogen concentration. If the WQ Module detects a concentration greater than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues

Ammonium Benthic $== K_{sed-O_2}^{NH_4}, \theta_{sed}^{NH_4}$

Model Construction: Section 4.7.3.3.1

Used in an inorganic nitrogen constituent model block to control the response of benthic ammonium flux to temperature and oxygen concentration.

$K_{sed-O_2}^{NH_4}$ - Sediment Half Saturation Oxygen Concentration for Ammonium Flux

Units	Range	Default
mg/L O ₂	(0, 4.8)	4
mmol/m ³ O ₂	(0, 150)	125

Science: Section E.1

The dissolved oxygen concentration for which the computed sediment ammonium flux is half the user specified rate, at 20°C. Cannot be varied spatially

$\theta_{sed}^{NH_4}$ - Sediment Ammonium Flux Temperature Coefficient

Default: 1

Units: NA

Range: (1, 1.1)

Science: Section E.1

The factor to which ($T-20$) is raised to account for temperature effects on ammonium sediment flux. A value of 1.0 will remove the effect of temperature

Ammonium Flux $== F_{sed}^{NH_4}$

Model Construction: Section 4.7.4

Used in a materials block to control the sediment flux rate of ammonium.

$F_{sed}^{NH_4}$ - Sediment Ammonium Flux

Units	Range	Default
mg NH ₄ -N/m ² /d	(0, 140)	0
mmol NH ₄ -N/m ² /d	(0, 10)	0

Science: Section [E.1](#)

The rate at which ammonium is exchanged between the sediments and overlying water column at 20°C excluding the influence of overlying dissolved oxygen concentration. Can be varied spatially via use of model mesh material types. This is not the maximum rate of ammonium sediment flux.

This parameter is output as a diagnostic variable. For further information, refer to [Ammonium User Defined Sediment Flux](#).

Ammonium Min Max == $[NH_4]_{min}^{NH_4}$, $[NH_4]_{max}^{NH_4}$

Model Construction: Section [4.7.3.3.1](#)

Used in an inorganic nitrogen constituent model block to set minimum and maximum ammonium concentrations.

$[NH_4]_{min}^{NH_4}$ - Minimum Ammonium Concentration

Units	Range	Default
mg/L NH ₄ -N	(0, 0.098)	NA
mmol/m ³ NH ₄ -N	(0, 7)	NA

Science: Appendix [E](#)

The minimum allowable ammonium concentration. If the WQ Module detects a concentration less than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues. A value other than zero for this parameter would be unusual

$[NH_4]_{max}^{NH_4}$ - Maximum Ammonium Concentration

Units	Range	Default
mg/L NH ₄ -N	(0, 98)	NA
mmol/m ³ NH ₄ -N	(0, 7000)	NA

Science: Appendix [E](#)

The maximum allowable ammonium concentration. If the WQ Module detects a concentration greater than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues

Anaerobic Oxidation of Ammonium == $k_{anmx}^{N_2}$, $K_{anmx-NH_4}^{N_2}$, $K_{anmx-NO_2}^{N_2}$

Model Construction: Section [4.7.3.3.1](#)

Used in an inorganic nitrogen constituent model block to control anaerobic oxidation of ammonium and its response to ambient ammonium and nitrate concentrations.

$k_{anmx}^{N_2}$ - Anaerobic Oxidation of Ammonium Rate

Units	Range	Default
mg N/L/d	(0, 0.5)	0
mmol N/m ³ /d	(0, 0.036)	0

Science: Section [E.4](#)

The rate at which ammonium is oxidised (consuming nitrite) to nitrogen gas N₂ at 20°C excluding the influence of ambient ammonium and nitrite concentrations. This is not solely a per day rate, but is the mass (or mmol) rate of production of nitrogen in free nitrogen gas, per unit volume, per day. Anammox only operates when ambient dissolved oxygen concentrations are less than 0.1 mg/L. A value of 0.0 will switch off anammox

 $K_{anmx-NH_4}^{N_2}$ - Half Saturation Ammonium Concentration for Anammox

Units	Range	Default
mg/L NH ₄ -N	(0, 10)	1.75
mmol/m ³ NH ₄ -N	(0, 714)	125

Science: Section [E.4](#)

The ammonium concentration for which the computed consumption of ammonium due to anaerobic oxidation would be half the corresponding anaerobic oxidation rate, excluding the influence of nitrite. Cannot be varied spatially

 $K_{anmx-NO_2}^{N_2}$ - Half Saturation Nitrite Concentration for Anammox

Units	Range	Default
mg/L NO ₂ -N	(0, 10)	1.75
mmol/m ³ NO ₂ -N	(0, 714)	125

Science: Section [E.4](#)

The nitrite concentration for which the computed consumption of ammonium due to anaerobic oxidation would be half the corresponding anaerobic oxidation rate, excluding the influence of ammonium. Cannot be varied spatially

Atmospheric Deposition

Navigation row for this command. Argument syntax depends on the selected implementation. Refer to the implementation specific sections immediately below.

Atmospheric Deposition == $[FRP]_{rain}$, $R_{atm-dry}^{FRPads}$

Model Construction: Section [4.7.3.4.1](#)

Used in an inorganic phosphorus constituent model block to control the wet (and dry) atmospheric deposition of FRP (adsorbed FRP).

$[FRP]_{rain}$ - FRP Concentration in Rainfall

Units	Range	Default
mg/L P	(0, 0.01)	0
mmol/m ³ P	(0, 0.32)	0

Science: Section 4.7.3.4.1

The concentration of FRP in rainfall which is directly deposited into the surface layer cells. If rainfall is modeled within TUFLOW FV, this will be computed from the mass flux values of rainfall

$R_{atm-dry}^{FRPads}$ - Dry Atmospheric Deposition Rate for Adsorbed FRP

Units	Range	Default
mg/m ² /d P	(0, 0.001)	0
mmol/m ² /d P	(0, 0.00003)	0

Science: Section 4.7.3.4.1

The dry atmospheric deposition rate of adsorbed FRP expressed as a flux per unit area per day. This flux is applied to the surface layer cells

Atmospheric Deposition == $[TN]_{rain}$, $R_{atm-dry}^{TN}$, $f_{TN}^{NO_3}$

Model Construction: Section 4.7.3.3.1

Used in an inorganic nitrogen constituent model block to control the wet and dry atmospheric deposition of inorganic nitrogen.

$[TN]_{rain}$ - Total Nitrogen Concentration in Rainfall

Units	Range	Default
mg/L N	(0, 1)	0
mmol/m ³ N	(0, 71)	0

Science: Section 4.7.3.3.1

The concentration of total nitrogen (NO₃ + NH₄) in rainfall which is directly deposited into the surface layer cells. The split between NO₃ and NH₄ is determined by $f_{TN}^{NO_3}$

$R_{atm-dry}^{TN}$ - Dry Atmospheric Deposition Rate for Total Nitrogen

Units	Range	Default
mg/m ² /d N	(0, 0.1)	0
mmol/m ² /d N	(0, 0.007)	0

Science: Section 4.7.3.3.1

The dry atmospheric deposition rate of total nitrogen (NO₃ + NH₄) expressed as a flux per unit area per day. This flux is applied to the surface layer cells. The split between NO₃ and NH₄ is determined by $f_{TN}^{NO_3}$

$f_{TN}^{NO_3}$ - Fraction of Atmospheric Total Nitrogen Deposited as Nitrate

Default: 0.5

Units: NA

Range: (0, 1)

Science: Section 4.7.3.3.1

The fraction of atmospheric nitrogen deposition (wet and dry) that is in the form of nitrate (NO₃), as opposed to ammonium (NH₄). The remainder is deposited as ammonium

Carbon Chl a Ratio == X_{cc}^{phy}

Model Construction: Section 4.7.3.5.1.10

Used in a phytoplankton constituent model block to set the mass of carbon per unit of chlorophyll *a* (Chl *a*).

X_{cc}^{phy} - Carbon to Chlorophyll A Ratio

Default: 40

Units: mg C/mg Chl *a*

Range: (1, 100)

Science: Section 6.2

The ratio of carbon to chlorophyll *a* in the cellular biomass of a phytoplankton group. The units of chlorophyll *a* in this ratio are milligrams (mg), not µg. This value is constant for a given phytoplankton group

Carbon Min Max == $[POC]_{min}^{POC}$, $[POC]_{max}^{POC}$, $[DOC]_{min}^{DOC}$, $[DOC]_{max}^{DOC}$

Model Construction: Section 4.8.3.5

Used in an organic matter constituent model block to set minimum and maximum particulate and dissolved organic carbon concentrations.

$[POC]_{min}^{POC}$ - Minimum POC Concentration

Units	Range	Default
mg/L C	(0, 0.1)	NA
mmol/m ³ C	(0, 8.33)	NA

Science: Appendix M

The minimum allowable labile particulate organic carbon concentration. If the WQ Module detects a concentration less than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues. A value other than zero for this parameter would be unusual

$[POC]_{max}^{POC}$ - Maximum POC Concentration

Units	Range	Default
mg/L C	(0, 100)	NA
mmol/m ³ C	(0, 8333)	NA

Science: Appendix M

The maximum allowable labile particulate organic carbon concentration. If the WQ Module detects a concentration greater than this, then it will be reset to this value, and reported in the WQ Module log file. The root

cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues

$[DOC]_{min}^{DOC}$ - Minimum DOC Concentration

Units	Range	Default
mg/L C	(0, 0.1)	NA
mmol/m ³ C	(0, 8.33)	NA

Science: Appendix [M](#)

The minimum allowable labile dissolved organic carbon concentration. If the WQ Module detects a concentration less than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues. A value other than zero for this parameter would be unusual

$[DOC]_{max}^{DOC}$ - Maximum DOC Concentration

Units	Range	Default
mg/L C	(0, 100)	NA
mmol/m ³ C	(0, 8333)	NA

Science: Appendix [M](#)

The maximum allowable labile dissolved organic carbon concentration. If the WQ Module detects a concentration greater than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues

cell water quality Depth == d_{min-wq}

Status: Optional

Model Construction: Section [4.4.1](#)

Instruct TUFLOW FV to not execute water quality calculations on cells that have depths less than this specified value.

d_{min-wq} - Minimum Water Quality Calculation Depth

Default: 0.01

Units: m

Range: (0, UD)

The minimum depth at which water calculations will be computed. This depth is the depth of the entire computational column that immediately overlies the sediment (bed) for a given 2D cell. The depth is specified in the TUFLOW FV control file

Denitrification

Navigation row for this command. Argument syntax depends on the selected implementation. Refer to the implementation specific sections immediately below.

Denitrification == Exponential, $R_{denit}^{NO_3}$, $K_{denit-O_2-exp}^{NO_3}$, $\theta_{denit}^{NO_3}$

Model Construction: Section 4.7.3.3.1

Used in an inorganic nitrogen constituent model block to activate the exponential model and control denitrification and its response to ambient oxygen concentrations and temperature.

For further information on the exponential denitrification model, refer to Section E.3.

$R_{denit}^{NO_3}$ - Denitrification Rate

Units	Range	Default
d	(0, 0.5)	0
		0

Science: Section E.3

The rate at which nitrate is denitrified to nitrogen gas N_2 at 20°C excluding the influence of ambient dissolved oxygen and nitrate concentrations. A value of 0.0 will switch off denitrification

$K_{denit-O_2-exp}^{NO_3}$ - Normalising Oxygen Concentration for Denitrification

Units	Range	Default
mg/L O_2	(0, 4.8)	4
mmol/m ³ O_2	(0, 150)	125

Science: Section E.3

The dissolved oxygen concentration that divides (normalises) the ambient dissolved oxygen concentration in the exponent term of the exponential denitrification model, at 20°C and with no influence of ambient nitrate concentration. This value is used if the 'exponential' denitrification model is specified as the first argument of the Denitrification command

$\theta_{denit}^{NO_3}$ - Denitrification Temperature Coefficient

Default: 1

Units: NA

Range: (1, 1.1)

Science: Section E.3

The factor to which $(T-20)$ is raised to account for temperature effects on denitrification. A value of 1.0 will remove the effect of temperature

Denitrification == Michaelis Menten, $R_{denit}^{NO_3}$, $K_{denit-O_2-MM}^{NO_3}$, $\theta_{denit}^{NO_3}$

Model Construction: Section 4.7.3.3.1

Used in an inorganic nitrogen constituent model block to activate the Michaelis Menten model and control denitrification and its response to ambient oxygen concentrations and temperature.

For further information on the Michaelis Menten denitrification model, refer to Section E.3.

$R_{denit}^{NO_3}$ - Denitrification Rate

Units	Range	Default
d	(0, 0.5)	0
		0

Science: Section [E.3](#)

The rate at which nitrate is denitrified to nitrogen gas N_2 at 20°C excluding the influence of ambient dissolved oxygen and nitrate concentrations. A value of 0.0 will switch off denitrification

$K_{denit-O_2-MM}^{NO_3}$ - Half Saturation Oxygen Concentration for Denitrification

Units	Range	Default
mg/L O_2	(0, 4.8)	4
mmol/m ³ O_2	(0, 150)	125

Science: Section [E.3](#)

The dissolved oxygen concentration for which the computed denitrification rate is half the user specified rate, at 20°C and with no influence of ambient nitrate concentration. This value is used if the ‘Michaelis Menten’ denitrification model is specified as the first argument of the Denitrification command

$\theta_{denit}^{NO_3}$ - Denitrification Temperature Coefficient

Default: 1

Units: NA

Range: (1, 1.1)

Science: Section [E.3](#)

The factor to which $(T-20)$ is raised to account for temperature effects on denitrification. A value of 1.0 will remove the effect of temperature

Disable water quality Model == $B_{disable-wq}$

Status: Optional

Model Construction: Section [4.4.1](#)

Instruct TUFLOW FV to disable (1) or enable (0) water quality calculations on all cells.

$B_{disable-wq}$ - Disable water quality calculation

Default: 0

Units: NA

Range: (0, 1)

A Boolean flag to disable (1) or enable (0) water quality calculations. The flag is specified in the TUFLOW FV control file

Diss Nitrate Reduction To Ammonium == $R_{DRNA}^{NO_3}$, $K_{DRNA-O_2}^{NO_3}$

Model Construction: Section [4.7.3.3.1](#)

Used in an inorganic nitrogen constituent model block to control dissimilatory reduction of nitrate to ammonium and its response to ambient oxygen concentrations.

$R_{DRNA}^{NO_3}$ - Dissimilatory Reduction of Nitrate to Ammonium Rate

Units	Range	Default
/d	(0, 0.05)	0
		0

Science: Section [E.5](#)

The rate at which nitrate is reduced to ammonium at 20°C excluding the influence of ambient nitrate concentrations. A value of 0.0 will switch off DRNA

$K_{DRNA-O_2}^{NO_3}$ - Half Saturation Oxygen Concentration for DRNA

Units	Range	Default
mg/L O ₂	(0, 10)	4
mmol/m ³ O ₂	(0, 312.5)	125

Science: Section [E.5](#)

The oxygen concentration for which the computed reduction of nitrate to ammonium would be half the corresponding rate. Cannot be varied spatially

DOC Flux == F_{sed}^{DOC}

Model Construction: Section [4.8.4](#)

Used in a materials block to control the sediment flux rate of DOC.

F_{sed}^{DOC} - Sediment DOC Flux

Units	Range	Default
mg C/m ² /d	(0, 120)	0
mmol C/m ² /d	(0, 10)	0

Science: Section [M.1](#)

The rate at which labile dissolved organic carbon is exchanged between the sediments and overlying water column at 20°C excluding the influence of overlying dissolved oxygen concentration. Can be varied spatially via use of model mesh material types. This is not the maximum rate of labile DOC sediment flux.

This parameter is output as a diagnostic variable. For further information, refer to [DOC User Defined Sediment Flux](#).

DON Flux == F_{sed}^{DON}

Model Construction: Section [4.8.4](#)

Used in a materials block to control the sediment flux rate of DON.

F_{sed}^{DON} - Sediment DON Flux

Units	Range	Default
mg N/m ² /d	(0, 21.126)	0
mmol N/m ² /d	(0, 1.509)	0

Science: Section [M.1](#)

The rate at which labile dissolved organic nitrogen is exchanged between the sediments and overlying water column at 20°C excluding the influence of overlying dissolved oxygen concentration. Can be varied spatially via use of model mesh material types. This is not the maximum rate of labile DON sediment flux.

This parameter is output as a diagnostic variable. For further information, refer to [DON User Defined Sediment Flux](#).

$$\text{DOP Flux} == F_{sed}^{DOP}$$

Model Construction: Section [4.8.4](#)

Used in a materials block to control the sediment flux rate of DOP.

F_{sed}^{DOP} - Sediment DOP Flux

Units	Range	Default
mg P/m ² /d	(0, 2.914)	0
mmol P/m ² /d	(0, 0.094)	0

Science: Section [M.1](#)

The rate at which labile dissolved organic phosphorus is exchanged between the sediments and overlying water column at 20°C excluding the influence of overlying dissolved oxygen concentration. Can be varied spatially via use of model mesh material types. This is not the maximum rate of labile DOP sediment flux.

This parameter is output as a diagnostic variable. For further information, refer to [DOP User Defined Sediment Flux](#).

[End Inorganic Nitrogen Model](#)

Model Construction: Section [4.7.3.3.1](#)

Used to terminate an inorganic nitrogen constituent model block. Must follow an [Inorganic Nitrogen Model](#) command.

[End Inorganic Phosphorus Model](#)

Model Construction: Section [4.7.3.4.1](#)

Used to terminate an inorganic phosphorus constituent model block. Must follow a [Inorganic Phosphorus Model](#) command.

[End Material](#)

Model Construction: Section [4.5.3](#)

Command to terminate a materials block. This command must be paired with a corresponding [Material](#) command to initiate the block.

End Organic Matter Model**Model Construction:** Section 4.8.3.5.1Used to terminate an organics constituent model block. Must follow an **Organic Matter Model** command.**End Oxygen Model****Model Construction:** Section 4.6.3.1.1Used to terminate an oxygen constituent model block. Must follow an **Oxygen Model** command.**End Pathogen Model****Status:** Conditional - Required if a pathogen constituent model is implemented via **Pathogen Model****Model Construction:** Section 4.6.3.2.1, Section 4.6.3.2.2**Required Dependent Command(s):** **Pathogen Model**Used to terminate a pathogen constituent model block. Must follow a **Pathogen Model** command.**End Phyto Model****Model Construction:** Section 4.7.3.5.1.13Used to terminate a phytoplankton constituent model block. Must follow a **Phyto Model** command.**End Silicate Model****Model Construction:** Section 4.7.3.2.1Used to terminate a silicate constituent model block. Must follow a **Silicate Model** command.**FRP Benthic** == $K_{sed-O_2}^{FRP}, \theta_{sed}^{FRP}$ **Model Construction:** Section 4.7.3.4.1

Used in an inorganic phosphorus constituent model block to control the response of benthic FRP flux to temperature and oxygen concentration.

 $K_{sed-O_2}^{FRP}$ - Sediment Half Saturation Oxygen Concentration for FRP Flux

Units	Range	Default
mg/L O ₂	(0, 4.8)	4
mmol/m ³ O ₂	(0, 150)	125

Science: Section F.1

The dissolved oxygen concentration for which the computed sediment FRP flux is half the user specified rate, at 20°C. Cannot be varied spatially

 θ_{sed}^{FRP} - Sediment FRP Flux Temperature Coefficient*Default:* 1*Units:* NA*Range:* (1, 1.1)*Science:* Section F.1The factor to which $(T-20)$ is raised to account for temperature effects on FRP sediment flux. A value of 1.0 will remove the effect of temperature

$$\text{FRP Flux} == F_{sed}^{FRP}$$

Model Construction: Section 4.7.4

Used in a materials block to control the sediment flux rate of FRP.

F_{sed}^{FRP} - Sediment FRP Flux

Units	Range	Default
mg FRP-P/m ² /d	(0, 155)	0
mmol FRP-P/m ² /d	(0, 5)	0

Science: Section F.1

The rate at which FRP is exchanged between the sediments and overlying water column at 20°C excluding the influence of overlying dissolved oxygen concentration. Can be varied spatially via use of model mesh material types. This is not the maximum rate of FRP sediment flux.

This parameter is output as a diagnostic variable. For further information, refer to [FRP User Defined Sediment Flux](#).

$$\text{FRP Min Max} == [FRP]_{min}^{FRP}, [FRP]_{max}^{FRP}$$

Model Construction: Section 4.7.3.4.1

Used in an inorganic phosphorus constituent model block to set minimum and maximum FRP concentrations.

$[FRP]_{min}^{FRP}$ - Minimum FRP Concentration

Units	Range	Default
mg/L PO ₄ -P	(0, 0.01)	NA
mmol/m ³ PO ₄ -P	(0, 0.32)	NA

Science: Appendix F

The minimum allowable FRP concentration. If the WQ Module detects a concentration less than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues. A value other than zero for this parameter would be unusual

$[FRP]_{max}^{FRP}$ - Maximum FRP Concentration

Units	Range	Default
mg/L PO ₄ -P	(0, 10)	NA
mmol/m ³ PO ₄ -P	(0, 320)	NA

Science: Appendix F

The maximum allowable FRP concentration. If the WQ Module detects a concentration greater than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues

FRPads Min Max == $[FRPads]_{min}^{FRPads}$, $[FRPads]_{max}^{FRPads}$

Model Construction: Section 4.7.3.4.2

Used in an inorganic phosphorus constituent model block to set minimum and maximum adsorbed FRP concentrations.

$[FRPads]_{min}^{FRPads}$ - Minimum Adsorbed FRP Concentration

Units	Range	Default
mg/L P	(0, 0.01)	NA
mmol/m ³ P	(0, 0.32)	NA

Science: Section 4.7.3.4.2

The minimum allowable adsorbed FRP concentration. If the WQ Module detects a concentration less than this, then it will be reset to this value, and reported in the WQ Module log file

$[FRPads]_{max}^{FRPads}$ - Maximum Adsorbed FRP Concentration

Units	Range	Default
mg/L P	(0, 1)	NA
mmol/m ³ P	(0, 32)	NA

Science: Section 4.7.3.4.2

The maximum allowable adsorbed FRP concentration. If the WQ Module detects a concentration greater than this, then it will be reset to this value, and reported in the WQ Module log file

Hydrolysis == R_{hyd}^{POC} , R_{hyd}^{PON} , R_{hyd}^{POP} , $K_{hyd-O_2}^{POM}$, θ_{hyd}^{POM}

Model Construction: Section 4.8.3.5.1

Used in an organics constituent model block to parameterise particulate organic carbon, nitrogen and phosphorus hydrolysis.

R_{hyd}^{POC} - POC Hydrolysis Rate

Units	Range	Default
/d	(0, 0.1)	0
		0

Science: Section M.2

The rate at which labile particulate organic carbon is hydrolysed to dissolved organic carbon at 20°C excluding the influence of ambient dissolved oxygen concentration. This is not the maximum rate of POC hydrolysis

R_{hyd}^{PON} - PON Hydrolysis Rate

Units	Range	Default
/d	(0, 0.015)	0
		0

Science: Section [M.2](#)

The rate at which labile particulate organic nitrogen is hydrolysed to dissolved organic nitrogen at 20°C excluding the influence of ambient dissolved oxygen concentration. This is not the maximum rate of PON hydrolysis

R_{hyd}^{POP} - POP Hydrolysis Rate

Units	Range	Default
/d	(0, 0.0009)	0
		0

Science: Section [M.2](#)

The rate at which labile particulate organic phosphorus is hydrolysed to dissolved organic phosphorus at 20°C excluding the influence of ambient dissolved oxygen concentration. This is not the maximum rate of POP hydrolysis

$K_{hyd-O_2}^{POM}$ - Half Saturation Oxygen Concentration for POM Hydrolysis

Units	Range	Default
mg/L O ₂	(0, 4.8)	4
mmol/m ³ O ₂	(0, 150)	125

Science: Section [M.2](#)

The dissolved oxygen concentration for which the computed hydrolysis of labile POM is half the user specified rate, at 20°C. Cannot be varied spatially. The same value is applied to all labile particulate organic constituents (carbon, nitrogen and phosphorus), and also to the breakdown of refractory particulate organic matter

θ_{hyd}^{POM} - POM Hydrolysis Temperature Coefficient

Default: 1

Units: NA

Range: (1, 1.1)

Science: Section [M.2](#)

The factor to which $(T-20)$ is raised to account for temperature effects on labile POM hydrolysis. A value of 1.0 will remove the effect of temperature. The same value is applied to all labile particulate organic constituents (carbon, nitrogen and phosphorus), and also to the breakdown of refractory particulate organic matter

Include Sediment == Include sediment transport calculations, Include sediment in density calculation

Status: Optional

Model Construction: Section [4.7.5.1.2](#)

TUFLOW FV command to include sediment simulation. Sediment must be simulated if adsorbed phosphorus is included in a WQ Module simulation.

Initial Condition 2D == Initial condition file name and path.csv

Status: Optional

Model Construction: Section 4.4.2.1

Ordered individual computed variable initial conditions in a columnar text file.

Initial Condition 3D == Initial condition file name and path.csv

Status: Optional

Model Construction: Section 4.4.2.1

Ordered individual computed variable initial conditions in a columnar text file.

Initial Scalar Profile == Initial condition file name and path.csv

Status: Optional

Model Construction: Section 4.4.2.1

Ordered individual computed variable initial conditions in a columnar text file.

Initial WQ Concentration == Comma separated WQ initial conditions

Status: Optional

Model Construction: Section 4.4.2.1

Ordered individual computed variable initial conditions.

Inorganic Nitrogen Model == AmmoniumNitrate

Model Construction: Section 4.7.3.3

Used to commence an inorganic nitrogen constituent model block via specification of a constituent model from the inorganic nitrogen constituent model class (Section 4.7.3.3).

Inorganic Phosphorus Model == FRPhs | FRPhsAds

Model Construction: Section 4.7.3.4

Used to commence an inorganic phosphorus constituent model block via specification of a constituent model (FRPhs or FRPhsAds) from the inorganic phosphorus constituent model class.

Light Limitation

Navigation row for this command. Argument syntax depends on the selected implementation. Refer to the implementation specific sections immediately below.

Light Limitation == Basic, Ke^{phy} , I_{K-bas}

Model Construction: Section 4.7.3.5.1.3

Used in a phytoplankton constituent model block to set basic light limitation parameters for the basic and advanced phytoplankton constituent models. If **Stokes Settling** is used, then the value of I_K specified in this command overrides any value specified using the **Settling** command.

For further information on the basic light limitation model, refer to Section 1.6.1.

Ke^{phy} – Phytoplankton Specific Shading Coefficient

Units	Range	Default
($\mu\text{g Chl } a/\text{L}$)/m	(0, 0.0225)	0
(mmol C/m ³)/m	(0, 0.01)	0

Science: Section [L.1](#)

The rate at which light is attenuated by phytoplankton. This coefficient is per unit concentration of phytoplankton, per metre (depth). It is multiplied by phytoplankton concentration in each computational cell to leave a value that has units of per meter, which is the same as standard extinction coefficients and therefore is able to be added to other (e.g. background) parallel extinction coefficients.

I_{K-bas} - Half Saturation Constant for Basic Model Light Growth Limitation

Default: 20

Units: W/m²

Range: (1, 1500)

Science: Section [I.6.1](#)

Used to compute the basic light limitation function for both basic and advanced phytoplankton constituent models. It divides (normalises) the photosynthetically available radiation incident on the top and bottom of a computational cell and forms the lower limit of the exponential integral

Light Limitation == Chalker, $K_{e^{phy}}$, I_{K-cha}

Model Construction: Section [4.7.3.5.1.3](#)

Used in a phytoplankton constituent model block to set Chalker light limitation parameters for the basic and advanced phytoplankton constituent models. If [Stokes Settling](#) is used then the value of I_K specified in this command overrides any value specified using the [Settling](#) command.

For further information on the chalker light limitation model, refer to Section [I.6.6](#).

$K_{e^{phy}}$ - Phytoplankton Specific Shading Coefficient

Units	Range	Default
($\mu\text{g Chl } a/\text{L}$)/m	(0, 0.0225)	0
(mmol C/m ³)/m	(0, 0.01)	0

Science: Section [L.1](#)

The rate at which light is attenuated by phytoplankton. This coefficient is per unit concentration of phytoplankton, per metre (depth). It is multiplied by phytoplankton concentration in each computational cell to leave a value that has units of per meter, which is the same as standard extinction coefficients and therefore is able to be added to other (e.g. background) parallel extinction coefficients.

I_{K-cha} - Half Saturation Constant for Chalker Model Light Growth Limitation

Default: 20

Units: W/m²

Range: (1, 1500)

Science: Section [I.6.6](#)

Used to compute the chalker light limitation function for both basic and advanced phytoplankton constituent models. It divides (normalises) the photosynthetically available radiation incident at the centre of a computational cell

Light Limitation == Integrated, Ke^{phy} , I_{S-int}

Model Construction: Section 4.7.3.5.1.3

Used in a phytoplankton constituent model block to set integrated light limitation parameters for the basic and advanced phytoplankton constituent models.

For further information on the integrated light limitation model, refer to Section 1.6.8.

Ke^{phy} - Phytoplankton Specific Shading Coefficient

Units	Range	Default
$/(μg\ Chl\ a/L)/m$	(0, 0.0225)	0
$/(mmol\ C/m^3)/m$	(0, 0.01)	0

Science: Section L.1

The rate at which light is attenuated by phytoplankton. This coefficient is per unit concentration of phytoplankton, per metre (depth). It is multiplied by phytoplankton concentration in each computational cell to leave a value that has units of per meter, which is the same as standard extinction coefficients and therefore is able to be added to other (e.g. background) parallel extinction coefficients.

I_{S-int} - Saturating Light Intensity for The Integrated Model Light Growth Limitation

Default: 20

Units: W/m^2

Range: (1, 1500)

Science: Section 1.6.8

Used to compute the integrated light limitation function for both basic and advanced phytoplankton constituent models. It divides (normalises) the photosynthetically available radiation incident on the top and bottom of a computational cell. This limitation function includes photoinhibition

Light Limitation == Jassby, Ke^{phy} , I_{K-jas}

Model Construction: Section 4.7.3.5.1.3

Used in a phytoplankton constituent model block to set Jassby light limitation parameters for the basic and advanced phytoplankton constituent models. If **Stokes Settling** is used then the value of I_K specified in this command overrides any value specified using the **Settling** command.

For further information on the Jassby light limitation model, refer to Section 1.6.5.

Ke^{phy} - Phytoplankton Specific Shading Coefficient

Units	Range	Default
$(μg\ Chl\ a/L)/m$	(0, 0.0225)	0
$(mmol\ C/m^3)/m$	(0, 0.01)	0

Science: Section L.1

The rate at which light is attenuated by phytoplankton. This coefficient is per unit concentration of phytoplankton, per metre (depth). It is multiplied by phytoplankton concentration in each computational cell to leave a value that has units of per meter, which is the same as standard extinction coefficients and therefore is able to be added to other (e.g. background) parallel extinction coefficients.

I_{K-jas} - Half Saturation Constant for Jassby Model Light Growth Limitation

Default: 20

Units: W/m²

Range: (1, 1500)

Science: Section [I.6.5](#)

Used to compute the jassby light limitation function for both basic and advanced phytoplankton constituent models. It divides (normalises) the photosynthetically available radiation incident at the centre of a computational cell

Light Limitation == `klepper`, Ke^{phy} , I_{S-kle}

Model Construction: Section [4.7.3.5.1.3](#)

Used in a phytoplankton constituent model block to set Klepper light limitation parameters for the basic and advanced phytoplankton constituent models.

For further information on the Klepper light limitation model, refer to Section [I.6.7](#).

Ke^{phy} - Phytoplankton Specific Shading Coefficient

Units	Range	Default
(μ g Chl <i>a</i> /L)/m	(0, 0.0225)	0
(mmol C/m ³)/m	(0, 0.01)	0

Science: Section [L.1](#)

The rate at which light is attenuated by phytoplankton. This coefficient is per unit concentration of phytoplankton, per metre (depth). It is multiplied by phytoplankton concentration in each computational cell to leave a value that has units of per meter, which is the same as standard extinction coefficients and therefore is able to be added to other (e.g. background) parallel extinction coefficients.

I_{S-kle} - Saturating Light Intensity for The Klepper Model Light Growth Limitation

Default: 20

Units: W/m²

Range: (1, 1500)

Science: Section [I.6.7](#)

Used to compute the klepper light limitation function for both basic and advanced phytoplankton constituent models. It divides (normalises) the photosynthetically available radiation incident at the centre of a computational cell. This limitation function includes photoinhibition

Light Limitation == `Monod`, Ke^{phy} , I_{K-mon}

Model Construction: Section [4.7.3.5.1.3](#)

Used in a phytoplankton constituent model block to set Monod light limitation parameters for the basic and advanced phytoplankton constituent models. If `Stokes Settling` is used, then the value of I_K specified in this command overrides any value specified using the `Settling` command.

For further information on the Monod light limitation model, refer to Section [I.6.2](#).

Ke^{phy} - Phytoplankton Specific Shading Coefficient

Units	Range	Default
($\mu\text{g Chl } a/\text{L}$)/m	(0, 0.0225)	0
(mmol C/m ³)/m	(0, 0.01)	0

Science: Section [L.1](#)

The rate at which light is attenuated by phytoplankton. This coefficient is per unit concentration of phytoplankton, per metre (depth). It is multiplied by phytoplankton concentration in each computational cell to leave a value that has units of per meter, which is the same as standard extinction coefficients and therefore is able to be added to other (e.g. background) parallel extinction coefficients.

I_{K-mon} - Half Saturation Constant for Monod Model Light Growth Limitation

Default: 20

Units: W/m²

Range: (1, 1500)

Science: Section [I.6.2](#)

Used to compute the monod light limitation function for both basic and advanced phytoplankton constituent models. It divides (normalises) the photosynthetically available radiation incident at the centre of a computational cell

Light Limitation == Steele, K_e^{phy} , I_{S-ste}

Model Construction: Section [4.7.3.5.1.3](#)

Used in a phytoplankton constituent model block to set Steele light limitation parameters for the basic and advanced phytoplankton constituent models.

For further information on the Steele light limitation model, refer to Section [I.6.3](#).

K_e^{phy} - Phytoplankton Specific Shading Coefficient

Units	Range	Default
($\mu\text{g Chl } a/\text{L}$)/m	(0, 0.0225)	0
(mmol C/m ³)/m	(0, 0.01)	0

Science: Section [L.1](#)

The rate at which light is attenuated by phytoplankton. This coefficient is per unit concentration of phytoplankton, per metre (depth). It is multiplied by phytoplankton concentration in each computational cell to leave a value that has units of per meter, which is the same as standard extinction coefficients and therefore is able to be added to other (e.g. background) parallel extinction coefficients.

I_{S-ste} - Saturating Light Intensity for The Steele Model Light Growth Limitation

Default: 20

Units: W/m²

Range: (1, 1500)

Science: Section [I.6.3](#)

Used to compute the steele light limitation function for both basic and advanced phytoplankton constituent models. It divides (normalises) the photosynthetically available radiation incident at the centre of a computational cell. This limitation function includes photoinhibition

Light Limitation == webb, $K e^{phy}$, I_{K-web}

Model Construction: Section 4.7.3.5.1.3

Used in a phytoplankton constituent model block to set Webb light limitation parameters for the basic and advanced phytoplankton constituent models. If **Stokes Settling** is used then the value of I_K specified in this command overrides any value specified using the **Settling** command.

For further information on the Webb light limitation model, refer to Section 1.6.4.

$K e^{phy}$ - Phytoplankton Specific Shading Coefficient

Units	Range	Default
($\mu\text{g Chl } a/\text{L}$)/m	(0, 0.0225)	0
(mmol C/m ³)/m	(0, 0.01)	0

Science: Section L.1

The rate at which light is attenuated by phytoplankton. This coefficient is per unit concentration of phytoplankton, per metre (depth). It is multiplied by phytoplankton concentration in each computational cell to leave a value that has units of per meter, which is the same as standard extinction coefficients and therefore is able to be added to other (e.g. background) parallel extinction coefficients.

I_{K-web} - Half Saturation Constant for Webb Model Light Growth Limitation

Default: 20

Units: W/m²

Range: (1, 1500)

Science: Section 1.6.4

Used to compute the webb light limitation function for both basic and advanced phytoplankton constituent models. It divides (normalises) the photosynthetically available radiation incident at the centre of a computational cell

Material == Up to 10 comma separated material integers

Model Construction: Section 4.5.3

Command to initiate a materials block. Commands within this block apply to the material numbers listed in this command.

Min Max == $[PHY]_{min}^{PHY}$, $[PHY]_{max}^{PHY}$

Model Construction: Section 4.7.3.5.1

Used in a phytoplankton constituent model block to set minimum and maximum phytoplankton group concentrations.

$[PHY]_{min}^{PHY}$ - Minimum Phyto Concentration

Units	Range	Default
$\mu\text{g/L Chl } a$	(0.01, 0.1)	0.01
mmol/m ³ C	(0.023, 0.225)	0.0225

Science: Appendix G

The minimum allowable group phytoplankton concentration. If the WQ Module detects a concentration less than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues. It is also important the this minimum value not be set to zero. If phytoplankton concentrations are allowed to reduce to zero then the numerical scheme will not allow the group to regrow because growth is applied as a multiplicative factor from one timestep to the next. Multiplying any growth rate by a previous timestep's zero group concentration will therefore always result in zero group concentration for subsequent timesteps

$[PHY]_{max}^{PHY}$ - Maximum Phyto Concentration

Units	Range	Default
$\mu\text{g/L Chl } a$	(0.01, 50)	NA
$\text{mmol/m}^3 \text{ C}$	(0.0025, 112.5)	NA

Science: Appendix G

The maximum allowable group phytoplankton concentration. If the WQ Module detects a concentration greater than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues

Mineralisation == R_{miner}^{DOM} , $K_{miner-O_2}^{DOM}$, θ_{miner}^{DOM} , f_{an} , $K_{miner-NO_3}^{NO_3}$

Model Construction: Section 4.8.3.5.1

Used in an organics constituent model block to parameterise dissolved organic matter (carbon, nitrogen and phosphorus) mineralisation. It includes the parameters that govern anaerobic mineralisation, that is, the consumption of nitrate in the dissolved organic matter mineralisation process.

R_{miner}^{DOM} - DOM Mineralisation Rate

Units	Range	Default
/d	(0, 0.1)	0
		0

Science: Section M.4

The rate at which labile dissolved organic carbon, nitrogen and phosphorus are mineralised to their corresponding dissolved inorganic constituents at 20°C excluding the influence of ambient dissolved oxygen concentration. This is not the maximum rate of mineralisation. The same rate is applied to all labile dissolved organic constituents (carbon, nitrogen and phosphorus)

$K_{miner-O_2}^{DOM}$ - Half Saturation Oxygen Concentration for DOM Mineralisation

Units	Range	Default
mg/L O_2	(0, 4.8)	4
$\text{mmol/m}^3 \text{ O}_2$	(0, 150)	125

Science: Section M.4

The dissolved oxygen concentration for which the computed aerobic and anaerobic mineralisation of labile DOM is half the user specified rate, at 20°C, and with f_{an} equal to 1.0. If f_{an} is equal to zero then this half saturation oxygen concentration is the dissolved oxygen concentration for which the computed aerobic mineralisation of labile DOM is half the user specified rate, again at 20°C. Cannot be varied spatially. The same value is applied to all labile dissolved organic constituents (carbon, nitrogen and phosphorus), and also to the activation of refractory dissolved organic carbon, nitrogen and phosphorus

θ_{miner}^{DOM} - DOM Mineralisation Temperature Coefficient

Default: 1

Units: NA

Range: (1, 1.1)

Science: Section [M.4](#)

The factor to which $(T-20)$ is raised to account for temperature effects on labile DOM mineralisation. A value of 1.0 will remove the effect of temperature. The same value is applied to all labile dissolved organic constituents (carbon, nitrogen and phosphorus), and also to the activation of refractory dissolved organic carbon, nitrogen and phosphorus

f_{an} - Anaerobic Mineralisation Multiplier

Default: 0

Units: NA

Range: (0, 1)

Science: Section [M.4](#)

The factor applied to the component of mineralisation of labile dissolved organic matter that does not consume dissolved oxygen. A value of 0.0 will entirely suppress the Michaelis-Menten weighting that non dissolved oxygen based processes have in calculating overall mineralisation of labile dissolved organic matter. Setting this parameter to zero does not suppress non dissolved oxygen mineralisation. This same factor is also applied to the activation of refractory dissolved organic carbon, nitrogen and phosphorus to their labile equivalents. If activation is to be simulated then the command [Mineralisation](#) will need to be issued to set f_{an} . In this case, and if the simulation of dissolved organic matter mineralisation is not desired, then set R_{miner}^{DOM} to be zero in the same mineralisation command

$K_{miner-NO_3}^{NO_3}$ - Half Saturation Nitrate Concentration for Nitrate Consumption via Anaerobic Mineralisation of Dissolved Organic Carbon

Units	Range	Default
mg/L NO ₃ -N	(0, 2.1)	1.75
mmol/m ³ NO ₃ -N	(0, 150)	125

Science: Section [M.4](#)

The nitrate concentration for which the computed consumption of nitrate due to anaerobic mineralisation is half the corresponding anaerobic mineralisation of labile dissolved organic carbon. If this parameter is set to zero, then the consumption of nitrate as a source of oxygen as part of organic matter mineralisation is switched off. Cannot be varied spatially

Mortality = k_d^{pth} , C_{SM}^{pth} , α , β , θ_{mor}^{pth}

Model Construction: Section [4.6.3.2.1](#)

Used in an (optional) pathogens constituent model block to control the mortality of pathogens. The fourth parameter β is unused but must be kept as a placeholder in this command so that five arguments are specified.

k_d^{pth} - Pathogen Dark Death Rate

Default: 0

Units: /d

Range: (0, 1)

Science: Section [N.1](#)

The natural mortality rate in freshwater at 20 °C. Also referred to as the dark death rate

C_{SM}^{pth} - Salinity Effect On Mortality

Default: 0

Units: /d /psu

Range: (0, 0.1)

Science: Section [N.1](#)

The salinity effect on mortality. Set this to zero to remove salinity effects on mortality

α - Parameter Controlling Salinity Mortality Dependence

Default: 1

Units: NA

Range: (0, 10)

Science: Section [N.1](#)

An exponentially applied controller of the mortality response to salinity. Set this to 1.0 to make salinity dependence linear. Do not set this and C_{SM}^{pth} to both be zero

β - Parameter Controlling DOC Trophic Mortality Dependence

Default: 1

Units: NA

Range: (0, 0)

Science: Section [N.1](#)

An exponentially applied controller of the mortality response to DOC. Not implemented

θ_{mor}^{pth} - Pathogen Mortality Temperature Coefficient

Default: 1

Units: NA

Range: (1, 1.2)

Science: Section [N.1](#)

The factor to which $(T-20)$ is raised to account for temperature effects on pathogen mortality. A value of 1.0 will remove the effect of temperature

Nitrate Benthic == $K_{sed-O_2}^{NO_3}$, $\theta_{sed}^{NO_3}$

Model Construction: Section [4.7.3.3.1](#)

Used in an inorganic nitrogen constituent model block to control the response of benthic nitrate flux to temperature and oxygen concentration.

$K_{sed-O_2}^{NO_3}$ - Sediment Half Saturation Oxygen Concentration for Nitrate Flux

Units	Range	Default
mg/L O ₂	(0, 4.8)	4
mmol/m ³ O ₂	(0, 150)	125

Science: Section [E.1](#)

The dissolved oxygen concentration for which the computed sediment nitrate flux is half the user specified rate, at 20°C. Cannot be varied spatially

$\theta_{sed}^{NO_3}$ - Sediment Nitrate Flux Temperature Coefficient

Default: 1

Units: NA

Range: (1, 1.1)

Science: Section [E.1](#)

The factor to which $(T-20)$ is raised to account for temperature effects on nitrate sediment flux. A value of 1.0 will remove the effect of temperature

Nitrate Flux == $F_{sed}^{NO_3}$

Model Construction: Section [4.7.4](#)

Used in a materials block to control the sediment flux rate of nitrate.

$F_{sed}^{NO_3}$ - Sediment Nitrate Flux

Units	Range	Default
mg NO ₃ -N/m ² /d	(0, 140)	0
mmol NO ₃ -N/m ² /d	(0, 10)	0

Science: Section [E.1](#)

The rate at which nitrate is exchanged between the sediments and overlying water column at 20°C excluding the influence of overlying dissolved oxygen concentration. Can be varied spatially via use of model mesh material types. This is not the maximum rate of nitrate sediment flux.

This parameter is output as a diagnostic variable. For further information, refer to [Nitrate User Defined Sediment Flux](#).

Nitrate Min Max == $[NO_3]_{min}^{NO_3}$, $[NO_3]_{max}^{NO_3}$

Model Construction: Section [4.7.3.3.1](#)

Used in an inorganic nitrogen constituent model block to set minimum and maximum nitrate concentrations.

$[NO_3]_{min}^{NO_3}$ - Minimum Nitrate Concentration

Units	Range	Default
mg/L NO ₃ -N	(0, 0.098)	NA
mmol/m ³ NO ₃ -N	(0, 7)	NA

Science: Appendix [E](#)

The minimum allowable nitrate concentration. If the WQ Module detects a concentration less than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues. A value other than zero for this parameter would be unusual

$[NO_3]_{max}^{NO_3}$ - Maximum Nitrate Concentration

Units	Range	Default
mg/L NO_3 -N	(0, 98)	NA
mmol/m ³ NO_3 -N	(0, 7000)	NA

Science: Appendix E

The maximum allowable nitrate concentration. If the WQ Module detects a concentration greater than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues

Nitrification == $R_{nitrif}^{NH_4}$, $K_{nitrif-O_2}^{NH_4}$, $\theta_{nitrif}^{NH_4}$

Model Construction: Section 4.7.3.3.1

Used in an inorganic nitrogen constituent model block to control nitrification and its response to oxygen concentration and temperature.

$R_{nitrif}^{NH_4}$ - Nitrification Rate

Units	Range	Default
/d	(0, 1)	0
		0

Science: Section E.2

The rate at which ammonium is nitrified to nitrate at 20°C excluding the influence of ambient dissolved oxygen concentration. A value of 0.0 will switch off nitrification

$K_{nitrif-O_2}^{NH_4}$ - Half Saturation Oxygen Concentration for Nitrification

Units	Range	Default
mg/L O_2	(0, 4.8)	4
mmol/m ³ O_2	(0, 150)	125

Science: Section E.2

The dissolved oxygen concentration for which the computed nitrification rate is half the user specified rate, at 20°C

$\theta_{nitrif}^{NH_4}$ - Nitrification Temperature Coefficient

Default: 1

Units: NA

Range: (1, 1.1)

Science: Section E.2

The factor to which $(T-20)$ is raised to account for temperature effects on nitrification. A value of 1.0 will remove the effect of temperature

Nitrogen Fixing == $R_{nfix}^{N_2}$, f_{nfix}^{phy}

Model Construction: Section 4.7.3.5.1.11

Used in a phytoplankton constituent model block to set the nitrogen fixing parameters of a phytoplankton constituent model. The first parameter sets the rate of nitrogen fixing and the second dictates the influence of nitrogen fixing on primary productivity.

$R_{nfix}^{N_2}$ - Nitrogen Fixing Rate

Units	Range	Default
mg N / mg Chl <i>a</i> / d	(0, 5)	0
mmol N / mmol C / d	(0, 0.16)	0

Science: Section J.2.3

The rate at which nitrogen N is fixed from the atmosphere to complement nitrogen uptake from the water column. This rate excludes the influence of nitrogen limitation due to water column nutrient scarcity. It is the mass (or molar) rate of uptake of nitrogen N from the atmosphere, not N₂. Note the units of chlorophyll *a* are in mg, not μ g

f_{nfix}^{phy} - Penalty Function of Nitrogen Fixing On Primary Productivity

Default: 1

Units: NA

Range: (0, 1)

Science: Section H.1

A rate modifier that accounts for the metabolic cost of nitrogen fixing on primary productivity. This modifier can be thought of as a penalty function, with values of zero and one corresponding to no and maximum penalties, respectively. A penalty of 1 (the default) will always set primary productivity to zero

Nitrogen Limitation

Navigation row for this command. Argument syntax depends on the selected implementation. Refer to the implementation specific sections immediately below.

Nitrogen Limitation == $[N]_{min}^{phy}$, K_{lim-N}^{phy}

Model Construction: Section 4.7.3.5.1.4

Used in a phytoplankton constituent model block to set nitrogen limitation parameters for the basic phytoplankton model.

$[N]_{min}^{phy}$ - Minimum Concentration of N for Phytoplankton Uptake

Units	Range	Default
mg/L N	(0, 0.1)	0.01
mmol/m ³ N	(0.00, 7.14)	0.71

Science: Section I.3.1

Used to compute the nitrogen limitation function in the basic phytoplankton model. Also used by the advanced phytoplankton model if internal nitrogen stores are exhausted. It is the minimum N concentration (as NH₄-N + NO₃-N) at which uptake of nitrogen by phytoplankton can occur

K_{lim-N}^{phy} - Half Saturation N Concentration for Phytoplankton Uptake of N

Units	Range	Default
mg/L N	(1, 5)	1
mmol/m ³ N	(71.4, 357.14)	71.43

Science: Section [I.3.1](#)

Used to compute the nitrogen limitation function in the basic phytoplankton model. Also used by the advanced phytoplankton model if internal nitrogen stores are exhausted. It is the concentration of N (NH₄-N + NO₃-N) that when added to the specified minimum $[N]_{min}^{phy}$ sets the nitrogen limitation function to a value of 0.5. A value of zero for this parameter will set the nitrogen limitation function to always be 1

Nitrogen Limitation == $[N]_{min}^{phy}$, K_{lim-N}^{phy} , $X_{N-C-min}^{phy}$, $X_{N-C-max}^{phy}$

Model Construction: Section [4.7.3.5.2.1](#)

Used in a phytoplankton constituent model block to set nitrogen limitation parameters for the advanced phytoplankton model.

$[N]_{min}^{phy}$ - Minimum Concentration of N for Phytoplankton Uptake

Units	Range	Default
mg/L N	(0, 0.1)	0.01
mmol/m ³ N	(0.00, 7.14)	0.71

Science: Section [I.3.1](#)

Used to compute the nitrogen limitation function in the basic phytoplankton model. Also used by the advanced phytoplankton model if internal nitrogen stores are exhausted. It is the minimum N concentration (as NH₄-N + NO₃-N) at which uptake of nitrogen by phytoplankton can occur

K_{lim-N}^{phy} - Half Saturation N Concentration for Phytoplankton Uptake of N

Units	Range	Default
mg/L N	(1, 5)	1
mmol/m ³ N	(71.4, 357.14)	71.43

Science: Section [I.3.1](#)

Used to compute the nitrogen limitation function in the basic phytoplankton model. Also used by the advanced phytoplankton model if internal nitrogen stores are exhausted. It is the concentration of N (NH₄-N + NO₃-N) that when added to the specified minimum $[N]_{min}^{phy}$ sets the nitrogen limitation function to a value of 0.5. A value of zero for this parameter will set the nitrogen limitation function to always be 1

$X_{N-C-min}^{phy}$ - Minimum Internal Nitrogen to Carbon Ratio of Phytoplankton

Default: 0.05

Units: mg N/mg C

Range: (0.02, 0.21)

Science: Section [I.3.2](#)

The minimum internal nitrogen to carbon ratio of phytoplankton before growth becomes limited by nitrogen. This forms the quota that is used to trigger increased nitrogen uptake

$X_{N-C-max}^{phy}$ - Maximum Internal Nitrogen to Carbon Ratio of Phytoplankton

Default: 0.20

Units: mg N/mg C

Range: (0.05, 0.30)

Science: Section [I.3.2](#)

The maximum internal nitrogen to carbon ratio of phytoplankton after which no further nitrogen uptake is allowed until growth dilutes the concentration

Nitrogen Min Max == $[PON]_{min}^{PON}$, $[PON]_{max}^{PON}$, $[DON]_{min}^{DON}$, $[DON]_{max}^{DON}$

Model Construction: Section [4.8.3.5](#)

Used in an organic matter constituent model block to set minimum and maximum particulate and dissolved organic nitrogen concentrations.

$[PON]_{min}^{PON}$ - Minimum PON Concentration

Units	Range	Default
mg/L N	(0, 0.01)	NA
mmol/m ³ N	(0, 0.71)	NA

Science: Appendix [M](#)

The minimum allowable labile particulate organic nitrogen concentration. If the WQ Module detects a concentration less than this, then it will be reset to this value, and reported in the WQ Module log file

$[PON]_{max}^{PON}$ - Maximum PON Concentration

Units	Range	Default
mg/L N	(0, 10)	NA
mmol/m ³ N	(0, 714)	NA

Science: Appendix [M](#)

The maximum allowable labile particulate organic nitrogen concentration. If the WQ Module detects a concentration greater than this, then it will be reset to this value, and reported in the WQ Module log file

$[DON]_{min}^{DON}$ - Minimum DON Concentration

Units	Range	Default
mg/L N	(0, 0.01)	NA
mmol/m ³ N	(0, 0.71)	NA

Science: Appendix [M](#)

The minimum allowable labile dissolved organic nitrogen concentration. If the WQ Module detects a concentration less than this, then it will be reset to this value, and reported in the WQ Module log file

$[DON]_{max}^{DON}$ - Maximum DON Concentration

Units	Range	Default
mg/L N	(0, 10)	NA
mmol/m ³ N	(0, 714)	NA

Science: Appendix [M](#)

The maximum allowable labile dissolved organic nitrogen concentration. If the WQ Module detects a concentration greater than this, then it will be reset to this value, and reported in the WQ Module log file

Organic Matter Model == Labile | Refractory

Model Construction: Section [4.8.3.5.1](#), Section [4.8.3.5.2](#)

Used to commence an organics constituent model block via specification of a model from the organics constituent model class.

Organics Benthic == $K_{sed-O_2}^{DOM}$, θ_{sed}^{DOM}

Model Construction: Section [4.8.3.5.1](#)

Used in an organics constituent model block to control the response of benthic DOM flux to temperature and oxygen concentration.

$K_{sed-O_2}^{DOM}$ - Sediment Half Saturation Oxygen Concentration for DOM Flux

Units	Range	Default
mg/L O ₂	(0, 4.8)	4
mmol/m ³ O ₂	(0, 150)	125

Science: Section [M.1](#)

The dissolved oxygen concentration for which the computed sediment labile DOM flux is half the user specified rate, at 20°C. Cannot be varied spatially. This value is applied equally to labile dissolved organic carbon, nitrogen and phosphorus

θ_{sed}^{DOM} - Sediment DOM Flux Temperature Coefficient

Default: 1

Units: NA

Range: (1, 1.1)

Science: Section [M.1](#)

The factor to which $(T-20)$ is raised to account for temperature effects on labile DOM sediment flux. A value of 1.0 will remove the effect of temperature. This value is applied equally to labile dissolved organic carbon, nitrogen and phosphorus

Oxygen

Navigation row for this command. Argument syntax depends on the selected implementation. Refer to the implementation specific sections immediately below.

oxygen == ON | OFF

Model Construction: Section [4.7.3.3.1](#)

Used in an inorganic nitrogen constituent model block to switch the dependence of all nitrogen (ammonium and nitrate) processes on dissolved oxygen ON or OFF.

For further information on the science of this command, refer to Section [E.1](#).

oxygen == ON | OFF

Model Construction: Section [4.8.3.5.1](#)

Used in an organics constituent model block to switch the dependence of all processes on dissolved oxygen ON or OFF. Anammox and DRNA processes will be switched off entirely if this command is issued and set to OFF.

For further information on the science of this command, refer to Section [M.1](#).

oxygen == ON | OFF

Model Construction: Section [4.7.3.4.1](#)

Used in an inorganic phosphorus constituent model block to switch the dependence of FRP processes on dissolved oxygen ON or OFF.

For further information on the science of this command, refer to Section [F.1](#).

oxygen == ON | OFF

Model Construction: Section [4.7.3.2.1](#)

Used in a silicate constituent model block to switch the dependence of silicate processes on dissolved oxygen 'ON' or 'OFF'.

For further information on the science of this command, refer to Section [D.1](#).

oxygen Benthic == $K_{sed-O_2}^{O_2}, \theta_{sed}^{O_2}$

Model Construction: Section [4.6.3.1.1](#)

Used in an oxygen constituent model block to control the response of benthic oxygen flux to temperature and oxygen concentration.

$K_{sed-O_2}^{O_2}$ - Sediment Half Saturation Oxygen Concentration for Oxygen Flux

Units	Range	Default
mg/L O ₂	(0, 4.8)	4
mmol/m ³ O ₂	(0, 150)	125

Science: Section [C.2](#)

The dissolved oxygen concentration for which the computed sediment oxygen flux is half the user specified rate, at 20°C. Cannot be varied spatially

$\theta_{sed}^{O_2}$ - Sediment Oxygen Flux Temperature Coefficient

Default: 1

Units: NA

Range: (1, 1.1)

Science: Section [C.2](#)

The factor to which $(T-20)$ is raised to account for temperature effects on oxygen sediment flux. A value of 1.0 will remove the effect of temperature

oxygen Flux == $F_{sed}^{O_2}$

Model Construction: Section [4.6.4](#)

Used in a materials block to control the sediment flux rate of oxygen.

$F_{sed}^{O_2}$ - Sediment Oxygen Flux

Units	Range	Default
mg O ₂ /m ² /d	(-6400, 0)	0
mmol O ₂ /m ² /d	(-200, 0)	0

Science: Section [C.2](#)

The rate at which dissolved oxygen is exchanged between the sediments and overlying water column at 20°C excluding the influence of overlying dissolved oxygen concentration. Can be varied spatially via use of model mesh material types. This is not the maximum rate of oxygen sediment flux.

This parameter is output as a diagnostic variable. For further information, refer to [Oxygen User Defined Sediment Flux](#).

oxygen Min Max == $[DO]_{min}^{O_2}, [DO]_{max}^{O_2}$

Model Construction: Section [4.6.3.1.1](#)

Used in an oxygen constituent model block to set minimum and maximum dissolved oxygen concentrations.

$[DO]_{min}^{O_2}$ - Minimum Dissolved Oxygen Concentration

Units	Range	Default
mg/L O ₂	(0, 0.5)	NA
mmol/m ³ O ₂	(0, 15.6)	NA

Science: Appendix [C](#)

The minimum allowable dissolved oxygen concentration. If the WQ Module detects a concentration less than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues. A value other than zero for this parameter would be unusual

$[DO]_{max}^{O_2}$ - Maximum Dissolved Oxygen Concentration

Units	Range	Default
mg/L O ₂	(6, 20)	NA
mmol/m ³ O ₂	(187.5, 625)	NA

Science: Appendix C

The maximum allowable dissolved oxygen concentration. If the WQ Module detects a concentration greater than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues

Oxygen Model == O2

Model Construction: Section 4.6.3.1, sec-ConModDOO2-4

Used to commence an oxygen constituent model block via specification of a constituent model from the oxygen constituent model class.

Oxygen Piston Model

Navigation row for this command. Argument syntax depends on the selected implementation. Refer to the implementation specific sections immediately below.

Oxygen Piston Model == Ho16

Model Construction: Section 4.6.3.1

Used in an oxygen constituent model block to activate the Ho et al 2016 oxygen piston model.

For further information on the science of this command, refer to Section C.1.

Oxygen Piston Model == wanninkhof92

Model Construction: Section 4.6.3.1

Used in an oxygen constituent model block to activate the Wanninkhof 1992 oxygen piston model.

For further information on the science of this command, refer to Section C.1.

Pathogen Model == Free | Attached, pathname

Status: Optional

Model Construction: Section 4.6.3.2.1, Section 4.6.3.2.2

Required Dependent Command(s): End Pathogen Model

Used to commence a pathogen model block via specification of a model from the pathogen constituent model class. pathname is any user specified pathgen group name that:

- Uses only alphanumeric characters
- Has no spaces
- Excludes the keyword 'PATH', and
- Is not the same as any other group name

Phosphorus Limitation == $[P]_{min}^{phy}$, K_{lim-P}^{phy}

Model Construction: Section 4.7.3.5.1.5

Used in a phytoplankton constituent model block to set phosphorus limitation parameters for the basic phytoplankton model.

$[P]_{min}^{phy}$ - Minimum Concentration of P for Phytoplankton Uptake

Units	Range	Default
mg/L P	(0, 0.1)	0.001
mmol/m ³ P	(0.0, 3.23)	0.03

Science: Section [I.4.1](#)

Used to compute the phosphorus limitation function in the basic phytoplankton model. Also used by the advanced phytoplankton model if internal phosphorus stores are exhausted. It is the minimum P concentration (as FRP-P) at which uptake of phosphorus by phytoplankton can occur

K_{lim-P}^{phy} - Half Saturation P Concentration for Phytoplankton Uptake of P

Units	Range	Default
mg/L P	(0.1, 0.5)	0.1
mmol/m ³ P	(3.23, 16.13)	3.23

Science: Section [I.4.1](#)

Used to compute the phosphorus limitation function in the basic phytoplankton model. Also used by the advanced phytoplankton model if internal phosphorus stores are exhausted. It is the concentration of P (FRP-P) that when added to the specified minimum $[P]_{min}^{phy}$ sets the phosphorus limitation function to a value of 0.5. A value of zero for this parameter will set the phosphorus limitation function to always be 1

Phosphorus Limitation == $[P]_{min}^{phy}$, K_{lim-P}^{phy} , $X_{P-C-min}^{phy}$, $X_{P-C-max}^{phy}$

Model Construction: Section [4.7.3.5.2.2](#)

Used in a phytoplankton constituent model block to set phosphorus limitation parameters for the advanced phytoplankton model.

$[P]_{min}^{phy}$ - Minimum Concentration of P for Phytoplankton Uptake

Units	Range	Default
mg/L P	(0, 0.1)	0.001
mmol/m ³ P	(0.0, 3.23)	0.03

Science: Section [I.4.1](#)

Used to compute the phosphorus limitation function in the basic phytoplankton model. Also used by the advanced phytoplankton model if internal phosphorus stores are exhausted. It is the minimum P concentration (as FRP-P) at which uptake of phosphorus by phytoplankton can occur

K_{lim-P}^{phy} - Half Saturation P Concentration for Phytoplankton Uptake of P

Units	Range	Default
mg/L P	(0.1, 0.5)	0.1
mmol/m ³ P	(3.23, 16.13)	3.23

Units	Range	Default
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Science: Section [I.4.1](#)

Used to compute the phosphorus limitation function in the basic phytoplankton model. Also used by the advanced phytoplankton model if internal phosphorus stores are exhausted. It is the concentration of P (FRP-P) that when added to the specified minimum $[P]_{min}^{phy}$ sets the phosphorus limitation function to a value of 0.5. A value of zero for this parameter will set the phosphorus limitation function to always be 1

$X_{P-C-min}^{phy}$ - Minimum Internal Phosphorus to Carbon Ratio of Phytoplankton

Default: 0.005

Units: mg P/mg C

Range: (0.003, 0.021)

Science: Section [I.4.2](#)

The minimum internal phosphorus to carbon ratio of phytoplankton before growth becomes limited by phosphorus. This forms the quota that is used to trigger increased phosphorus uptake

$X_{P-C-max}^{phy}$ - Maximum Internal Phosphorus to Carbon Ratio of Phytoplankton

Default: 0.020

Units: mg P/mg C

Range: (0.005, 0.030)

Science: Section [I.4.2](#)

The maximum internal phosphorus to carbon ratio of phytoplankton after which no further phosphorus uptake is allowed until growth dilutes the concentration

Phosphorus Min Max == $[POP]_{min}^{POP}$, $[POP]_{max}^{POP}$, $[DOP]_{min}^{DOP}$, $[DOP]_{max}^{DOP}$

Model Construction: Section [4.8.3.5](#)

Used in an organic matter constituent model block to set minimum and maximum particulate and dissolved organic phosphorus concentrations.

$[POP]_{min}^{POP}$ - Minimum POP Concentration

Units	Range	Default
mg/L P	(0, 0.001)	NA
mmol/m ³ P	(0, 0.032)	NA

Science: Appendix [M](#)

The minimum allowable labile particulate organic phosphorus concentration. If the WQ Module detects a concentration less than this, then it will be reset to this value, and reported in the WQ Module log file

$[POP]_{max}^{POP}$ - Maximum POP Concentration

Units	Range	Default
mg/L P	(0, 1)	NA
mmol/m ³ P	(0, 32)	NA

Science: Appendix M

The maximum allowable labile particulate organic phosphorus concentration. If the WQ Module detects a concentration greater than this, then it will be reset to this value, and reported in the WQ Module log file

$[DOP]_{min}^{DOP}$ - Minimum DOP Concentration

Units	Range	Default
mg/L P	(0, 0.001)	NA
mmol/m ³ P	(0, 0.032)	NA

Science: Appendix M

The minimum allowable labile dissolved organic phosphorus concentration. If the WQ Module detects a concentration less than this, then it will be reset to this value, and reported in the WQ Module log file

$[DOP]_{max}^{DOP}$ - Maximum DOP Concentration

Units	Range	Default
mg/L P	(0, 1)	NA
mmol/m ³ P	(0, 32)	NA

Science: Appendix M

The maximum allowable labile dissolved organic phosphorus concentration. If the WQ Module detects a concentration greater than this, then it will be reset to this value, and reported in the WQ Module log file

Phyto Model == Basic | Advanced, group_name

Model Construction: Section 4.7.3.5

Used to commence a phytoplankton constituent model block via specification of a model from the phytoplankton constituent model class (Basic or Advanced), and a phytoplankton 'group_name'. The group name can be any name required. If the advanced phytoplankton model is used then internal nitrogen and phosphorus concentrations will be simulated as computed variables and therefore must have respective initial conditions and boundary conditions specified, paying attention to ordering rules as required.

Primary Productivity == R_{prod}^{phy} , θ_{prod}^{phy}

Model Construction: Section 4.7.3.5.1.8

Used in a phytoplankton constituent model block to set primary productivity parameters of a phytoplankton constituent model.

R_{prod}^{phy} - Phytoplankton Primary Productivity Rate

Default: 0

Units: /d

Range: (0, 3.5)

Science: Section H.1

The phytoplankton primary productivity (growth) rate at 20°C with no light, temperature, salinity, silicate or nutrient limitation. This rate is multiplied by ambient phytoplankton concentration to derive initial carbon, nutrient and silicate uptake fluxes

θ_{prod}^{phy} - Phytoplankton Primary Productivity Temperature Coefficient

Default: 1

Units: NA

Range: (1, 1.1)

Science: Section [1.2.2](#)

The factor to which $(T-20)$ is raised to account for temperature effects on phytoplankton growth in the standard temperature limitation function. A value of 1.0 will remove the effect of temperature

Ref Activation == R_{act}^{RDOM}

Model Construction: Section [4.8.3.5.2](#)

Used in an organic matter constituent model block to set the rate of activation of refractory dissolved organic carbon, nitrogen and phosphorus.

R_{act}^{RDOM} - RDOM Activation Rate

Units	Range	Default
/d	(0, 0.1)	0
		0

Science: Section [M.5](#)

The rate at which refractory dissolved organic carbon, nitrogen and phosphorus are activated to their corresponding labile dissolved organic constituents at 20°C excluding the influence of ambient dissolved oxygen concentration. This is not the maximum rate of activation. The same rate is applied to all refractory dissolved organic constituents (carbon, nitrogen and phosphorus)

Ref Breakdown == R_{bdn}^{RPOM} , X_N^{RPOM} , X_P^{RPOM}

Model Construction: Section [4.8.3.5.2](#)

Used in an organics constituent model block to parameterise the breakdown of refractory particulate organic matter.

R_{bdn}^{RPOM} - RPOM Breakdown Rate

Units	Range	Default
/d	(0, 0.1)	0
		0

Science: Section [M.3](#)

The rate at which refractory particulate organic matter (a single computed variable) is broken down to labile particulate organic carbon, nitrogen and phosphorus (three computed variables) at 20°C excluding the influence of ambient dissolved oxygen concentration. This is not the maximum rate of breakdown

X_N^{RPOM} - Ratio of N to C in Refractory Particulate Organic Matter

Default: 0.15

Units: NA

Range: (0.094, 0.19)

Science: Section [M.3](#)

The molar ratio of N to C in refractory particulate organic matter. This ratio should not differ significantly from the Redfield ratio of 16/106.

X_P^{RPOM} - Ratio of P to C in Refractory Particulate Organic Matter

Default: 0.0094

Units: NA

Range: (0.00094, 0.019)

Science: Section [M.3](#)

The molar ratio of P to C in refractory particulate organic matter. This ratio should not differ significantly from the Redfield ratio of 1/106.

Ref Carbon Min Max == $[RPOM]_{min}^{RPOM}$, $[RPOM]_{max}^{RPOM}$, $[RDOC]_{min}^{RDOC}$, $[RDOC]_{max}^{RDOC}$

Model Construction: Section [4.8.3.5.2](#)

Used in an organic matter constituent model block to set minimum and maximum refractory particulate organic matter and refractory dissolved organic carbon concentrations.

$[RPOM]_{min}^{RPOM}$ - Minimum RPOM Concentration

Units	Range	Default
mg/L C	(0, 0.1)	NA
mmol/m ³ C	(0, 8.33)	NA

Science: Appendix [M](#)

The minimum allowable refractory particulate organic matter concentration. Although referred to as organic matter, it is accounted as (and in units of) carbon in the WQ Module. If the WQ Module detects a concentration less than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues. A value other than zero for this parameter would be unusual

$[RPOM]_{max}^{RPOM}$ - Maximum RPOM Concentration

Units	Range	Default
mg/L C	(0, 100)	NA
mmol/m ³ C	(0, 8333)	NA

Science: Appendix [M](#)

The maximum allowable refractory particulate organic matter concentration. Although referred to as organic matter, it is accounted as (and in units of) carbon in the WQ Module. If the WQ Module detects a concentration greater than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues

$[RDOC]_{min}^{RDOC}$ - Minimum RDOC Concentration

Units	Range	Default
mg/L C	(0, 0.1)	NA

Units	Range	Default
mmol/m ³ C	(0, 8.33)	NA

Science: Appendix [M](#)

The minimum allowable refractory dissolved organic carbon concentration. If the WQ Module detects a concentration less than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues. A value other than zero for this parameter would be unusual

$[RDOC]_{max}^{RDOC}$ - Maximum RDOC Concentration

Units	Range	Default
mg/L C	(0, 100)	NA
mmol/m ³ C	(0, 8333)	NA

Science: Appendix [M](#)

The maximum allowable refractory dissolved organic carbon concentration. If the WQ Module detects a concentration greater than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues

Ref Nitrogen Min Max == $[RDON]_{min}^{RDON}$, $[RDON]_{max}^{RDON}$

Model Construction: Section [4.8.3.5.2](#)

Used in an organic matter constituent model block to set minimum and maximum refractory dissolved organic nitrogen concentrations.

$[RDON]_{min}^{RDON}$ - Minimum RDON Concentration

Units	Range	Default
mg/L N	(0, 0.1)	NA
mmol/m ³ N	(0, 7.14)	NA

Science: Appendix [M](#)

The minimum allowable refractory dissolved organic nitrogen concentration. If the WQ Module detects a concentration less than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues. A value other than zero for this parameter would be unusual

$[RDON]_{max}^{RDON}$ - Maximum RDON Concentration

Units	Range	Default
mg/L N	(0, 100)	NA
mmol/m ³ N	(0, 7143)	NA

Science: Appendix M

The maximum allowable refractory dissolved organic nitrogen concentration. If the WQ Module detects a concentration greater than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues

Ref Phosphorus Min Max == $[RDOP]_{min}^{RDOP}$, $[RDOP]_{max}^{RDOP}$

Model Construction: Section 4.8.3.5.2

Used in an organic matter constituent model block to set minimum and maximum refractory dissolved organic phosphorus concentrations.

$[RDOP]_{min}^{RDOP}$ - Minimum RDOP Concentration

Units	Range	Default
mg/L P	(0, 0.01)	NA
mmol/m ³ P	(0, 0.32)	NA

Science: Appendix M

The minimum allowable refractory dissolved organic phosphorus concentration. If the WQ Module detects a concentration less than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues. A value other than zero for this parameter would be unusual

$[RDOP]_{max}^{RDOP}$ - Maximum RDOP Concentration

Units	Range	Default
mg/L P	(0, 10)	NA
mmol/m ³ P	(0, 323)	NA

Science: Appendix M

The maximum allowable refractory dissolved organic phosphorus concentration. If the WQ Module detects a concentration greater than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues

Ref Photolysis == f_{photo}^{RDOM}

Model Construction: Section 4.8.3.5.2

Used in an organics constituent model block to parameterise the proportion of photolysis of refractory dissolved organic matter that produces labile dissolved organic matter.

f_{photo}^{RDOM} - RDOM Photolysis Fraction

Default: 0

Units: NA

Range: (0, 1)

Science: Section M.6

The proportion of photolysed refractory dissolved organic matter that is converted to labile dissolved organic matter. The remaining proportion is converted to dissolved inorganic carbon and nutrients. This multiplier is applied equally to refractory dissolved organic carbon, nitrogen and phosphorus

Ref Self Shading == Ke^{RPOM} , R_{CDOM}^{RDOM}

Model Construction: Section 4.8.3.5.2

Used in an organics constituent model block to parameterise light attenuation due to the presence of refractory particulate and dissolved organic matter.

Ke^{RPOM} – RPOM Specific Shading Coefficient

Units	Range	Default
/(mg RPOM/L)/m	(0, 8.33)	0
/(mmol RPOM/m ³)/m	(0, 0.1)	0

Science: Section M.7

The rate at which light is attenuated by refractory particulate organic matter. This coefficient is per unit concentration of refractory particulate organic carbon (the units of RPOM) per metre (depth). It is multiplied by RPOM concentration in each computational cell to leave a value that has units of per meter, which is the same as standard extinction coefficients and therefore is able to be added to other (e.g. background) parallel extinction coefficients

R_{CDOM}^{RDOM} – CDOM Multiplier

Default: 0

Units: NA

Range: (0, 2)

Science: Section M.7

The linear multiplicative factor applied to the calculated value of CDOM for use in organic matter self shading calculations. A value greater (less) than 1.0 increases (decreases) the CDOM estimate and hence increases (decreases) shading. . This coefficient is dimensionless but can be thought of as light attenuation per unit of CDOM, which are both in units of /m. Multiplying this parameter by CDOM in each computational cell therefore leaves a value that has units of per meter, which is the same as standard extinction coefficients and therefore is able to be added to other (e.g. background) parallel extinction coefficients

Ref Settling

Navigation row for this command. Argument syntax depends on the selected implementation. Refer to the implementation specific sections immediately below.

Ref Settling == Constant, V_{settle}^{rorg}

Model Construction: Section 4.8.3.5.2

Used in an organic matter constituent model block to control the settling rate of refractory particulate organic matter. This will be linked directly to the TUFLOW FV ST Module in future releases of the WQ Module.

For further information on the constant settling model, refer to Section M.8.2.

V_{settle}^{rorg} - Refractory Organic Matter Settling Velocity

Default: 0

Units: m/d

Range: (-50, 0)

Science: Section [M.8.2](#)

The settling velocity applied to refractory particulate organic matter for constant or density related settling calculations. A negative value is a downwards velocity. Future releases of the WQ Module will dynamically link settling velocity to calculations made by the TUFLOW FV ST Module

Ref Settling == None

Model Construction: Section [4.8.3.5.2](#)

Used in an organic matter constituent model block to set the settling rate of refractory particulate organic matter to zero.

For further information on the science of this command, refer to Section [M.8.1](#).

Ref Settling == Stokes, d_{rorg} , ρ_{rorg}

Model Construction: Section [4.8.3.5.2](#)

Used in an organic matter constituent model block to control the settling rate of refractory particulate organic matter. This will be linked directly to the TUFLOW FV ST Module in future releases of the WQ Module.

For further information on the stokes settling model, refer to Section [M.8.4](#).

d_{rorg} - Refractory Organic Matter Stokes Diameter

Default: 1 e-09

Units: m

Range: (1 e-09, 1 e -06)

Science: Section [M.8.4](#)

The conceptual diameter of refractory particulate organic matter applied in stokes calculations of settling velocity. Future releases of the WQ Module will dynamically link settling velocity to calculations made by the TUFLOW FV ST Module

ρ_{rorg} - Refractory Organic Matter Stokes Density

Default: 2000

Units: kg/m³

Range: (1000, 3000)

Science: Section [M.8.4](#)

The density of refractory particulate organic matter applied in stokes calculations of settling velocity. Future releases of the WQ Module will dynamically link settling velocity to calculations made by the TUFLOW FV ST Module

Ref Settling == Thermal, V_{settle}^{rorg}

Model Construction: Section [4.8.3.5.2](#)

Used in an organic matter constituent model block to control the settling rate of refractory particulate organic matter. This will be linked directly to the TUFLOW FV ST Module in future releases of the WQ Module.

For further information on the thermal settling model, refer to Section [M.8.3](#).

V_{settle}^{org} - Refractory Organic Matter Settling Velocity

Default: 0

Units: m/d

Range: (-50, 0)

Science: Section [M.8.2](#)

The settling velocity applied to refractory particulate organic matter for constant or density related settling calculations. A negative value is a downwards velocity. Future releases of the WQ Module will dynamically link settling velocity to calculations made by the TUFLOW FV ST Module

Report Min Max Warnings == ON | OFF

Model Construction: Section [4.5.1](#)

Used in Part 1: Simulation controls of WQ Module control file to suppress writing concentration limit exceedance warnings to the WQ log file. If not specified it is set to on. This command should not be used as a way to ignore concentration exceedances, and has only been included in the WQ Module to allow for the rare occasions when known and expected exceedances occur regularly - writing of these to the log file can cause very large log files to be written and result in system instability.

Respiration == R_{resp}^{phy} , θ_{resp}^{phy} , $f_{true-resp}^{phy}$, $f_{excr-loss}^{phy}$, f_{exud}^{phy}

Model Construction: Section [4.7.3.5.1.9](#)

Used in a phytoplankton constituent model block to set respiration and exudation parameters of a phytoplankton constituent model.

R_{resp}^{phy} - Phytoplankton Respiration Rate

Default: 0

Units: /d

Range: (0, 0.1)

Science: Section [H.2](#)

The phytoplankton respiration rate at 20°C with no temperature or salinity limitation. This rate is multiplied by ambient phytoplankton concentration to derive excretion and mortality fluxes. It is added to the parallel primary productivity and exudation rates and then multiplied by ambient phytoplankton concentration to compute biomass flux

θ_{resp}^{phy} - Phytoplankton Respiration Temperature Coefficient

Default: 1

Units: NA

Range: (1, 1.1)

Science: Section [H.2](#)

The factor to which $(T-20)$ is raised to account for temperature effects on phytoplankton respiration. A value of 1.0 will remove the effect of temperature

$f_{true-resp}^{phy}$ - Fraction of Phytoplankton Respiration That Is True Respiration

Default: 1

Units: NA

Range: (0, 1)

Science: Section [K.1](#)

The proportion of consumed carbohydrates (that were generated during photosynthesis) that are converted to energy, as opposed to waste matter. A value of one (zero) has all consumed carbohydrates converted to energy (waste), and will minimise (maximise) excretive losses

$f_{excr-loss}^{phy}$ - Fraction of Phytoplankton Loss That Is Excretion

Default: 0

Units: NA

Range: (0, 1)

Science: Section [K.1](#)

The proportion of combined excretive and mortality losses that are excretive. If $f_{true-resp}^{phy}$ is set to one (zero) then this parameter has no (maximum) effect.

f_{exud}^{phy} - Fraction of Primary Production Lost to Exudation

Default: 0

Units: NA

Range: (0, 1)

Science: Section [H.3](#)

The proportion of primary production that does not generate retained cellular carbon biomass, but is lost through exudation (and hence excretion). Exudation losses are summed with potentially modified respiration losses to compute excretion

Restart == Restart file path and name.rst

Status: Optional

Model Construction: Section [4.4.2.1](#)

Specification of full path and name of previously saved restart file.

Salinity Limitation

Navigation row for this command. Argument syntax depends on the selected implementation. Refer to the implementation specific sections immediately below.

Salinity Limitation == Estuarine, $S_{opt-est}^{phy}$, $S_{max-est}^{phy}$, P_{est}^{phy}

Model Construction: Section [4.7.3.5.1.2](#)

Used in a phytoplankton constituent model block to select the estuarine phytoplankton group salinity limitation.

For further information on the estuarine salinity limitation model, refer to Section [1.7.5](#).

$S_{opt-est}^{phy}$ - Optimum Estuarine Salinity

Default: 0

Units: g/L

Range: (0, 45)

Science: Section [1.7.5](#)

Used to compute the estuarine salinity limitation function. It is the salinity at which the estuarine salinity limitation function has a value of 1

$S_{max-est}^{phy}$ - Maximum Estuarine Salinity

Default: 5

Units: g/L

Range: (0, 45)

Science: Section [1.7.5](#)

Used to compute the estuarine salinity limitation function. It is the maximum salinity at which the estuarine salinity limitation function has a value greater than zero

P_{est}^{phy} - Power Coefficient for Estuarine Salinity Limitation

Default: 0

Units: NA

Range: (0, 5)

Science: Section [1.7.5](#)

Used to compute the estuarine salinity limitation function. It determines the gradient of the estuarine limitation function (with salinity) above and below $S_{opt-est}^{phy}$. Small (large) values of this parameter provide low (high) gradients

Salinity Limitation == Fresh, $S_{opt-fresh}^{phy}$, $S_{max-fresh}^{phy}$, $L_{max-fresh}^{phy}$

Model Construction: Section [4.7.3.5.1.2](#)

Used in a phytoplankton constituent model block to select the freshwater phytoplankton group salinity limitation.

For further information on the freshwater salinity limitation model, refer to Section [1.7.2](#).

$S_{opt-fresh}^{phy}$ - Optimum Freshwater Salinity

Default: 0

Units: g/L

Range: (0, 45)

Science: Section [1.7.2](#)

Used to compute the freshwater salinity limitation function. It is the maximum salinity at which the freshwater salinity limitation function has a value of 1

$S_{max-fresh}^{phy}$ - Maximum Freshwater Salinity

Default: 5

Units: g/L

Range: (0, 45)

Science: Section [1.7.2](#)

Used to compute the freshwater salinity limitation function. It is the maximum salinity at which the freshwater salinity limitation function is greater than the value of $L_{max-fresh}^{phy}$

$L_{max-fresh}^{phy}$ - Limitation Function At Maximum Freshwater Salinity

Default: 0

Units: NA

Range: (0, -)

Science: Section [1.7.2](#)

Used to compute the freshwater salinity limitation function. It is the value of the freshwater limitation function at a salinity of $S_{max-fresh}$. If this limitation function value is set to be between zero and one (greater than one), then the computed limitation will be applied as a reductive (enhancement) factor to primary productivity (respiration).

Salinity Limitation == Marine, $S_{opt-marine}^{phy}$, $L_{zero-marine}^{phy}$

Model Construction: Section [4.7.3.5.1.2](#)

Used in a phytoplankton constituent model block to select the marine phytoplankton group salinity limitation.

For further information on the marine salinity limitation model, refer to Section [1.7.3](#).

$S_{opt-marine}^{phy}$ - Optimum Marine Salinity

Default: 0

Units: g/L

Range: (0, 45)

Science: Section [I.7.3](#)

Used to compute the marine salinity limitation function. It is the minimum salinity at which the marine salinity limitation function has a value of 1

$L_{zero-marine}^{phy}$ - Limitation Function At Zero Marine Salinity

Default: 0

Units: NA

Range: (0, -)

Science: Section [I.7.3](#)

Used to compute the marine salinity limitation function. It is the value of the marine limitation function at a salinity of zero. If this limitation function value is set to be between zero and one (greater than one), then the computed limitation will be applied as a reductive (enhancement) factor to primary productivity (respiration).

Salinity Limitation == Mixed, $S_{opt-mix}^{phy}$, $S_{max-mix}^{phy}$, $L_{zero-mix}^{phy}$

Model Construction: Section [4.7.3.5.1.2](#)

Used in a phytoplankton constituent model block to select the mixed phytoplankton group salinity limitation.

For further information on the mixed salinity limitation model, refer to Section [I.7.4](#).

$S_{opt-mix}^{phy}$ - Optimum Mixed Salinity

Default: 0

Units: g/L

Range: (0, 45)

Science: Section [I.7.4](#)

Used to compute the mixed salinity limitation function. It is the minimum salinity at which the mixed salinity limitation function has a value of 1

$S_{max-mix}^{phy}$ - Maximum Mixed Salinity

Default: 5

Units: g/L

Range: (0, 45)

Science: Section [I.7.4](#)

Used to compute the mixed salinity limitation function. It is the maximum salinity at which the mixed salinity limitation function has a value of 1

$L_{zero-mix}^{phy}$ - Limitation Function At Zero And ($S_{Opt-Mix}^{phy} + S_{Max-Mix}^{phy}$) Mixed Salinity

Default: 0

Units: NA

Range: (0, -)

Science: Section [I.7.4](#)

Used to compute the mixed salinity limitation function. It is the value of the mixed limitation function at a salinity of zero and ($S_{opt-mix}^{phy} + S_{max-mix}^{phy}$). If this limitation function value is set to be between zero and one (greater than one), then the computed limitation will be applied as a reductive (enhancement) factor to primary productivity (respiration).

Salinity Limitation == None

Model Construction: Section [4.7.3.5.1.2](#)

Used in a phytoplankton constituent model block to turn off phytoplankton group salinity limitation.

For more information on the science of this command, refer to Section [I.7.1](#).

Self Shading == K_e^{POM} , K_e^{DOM}

Model Construction: Section [4.8.3.5.1](#)

Used in an organics constituent model block to parameterise light attenuation due to the presence of particulate and dissolved organic matter.

K_e^{POM} - POM Specific Shading Coefficient

Units	Range	Default
/(mg POC/L)/m	(0, 8.33)	0
/(mmol POC/m ³)/m	(0, 0.1)	0

Science: Section [M.7](#)

The rate at which light is attenuated by labile particulate organic matter. This coefficient is per unit concentration of particulate organic carbon (which is used as a proxy for particulate organic matter) per metre (depth). It is multiplied by POC concentration in each computational cell to leave a value that has units of per meter, which is the same as standard extinction coefficients and therefore is able to be added to other (e.g. background) parallel extinction coefficients

K_e^{DOM} - DOM Specific Shading Coefficient

Units	Range	Default
/(mg DOC/L)/m	(0, 8.33)	0
/(mmol DOC/m ³)/m	(0, 0.1)	0

Science: Section [M.7](#)

The rate at which light is attenuated by labile dissolved organic matter. This coefficient is per unit concentration of dissolved organic carbon (which is used as a proxy for dissolved organic matter) per metre (depth). It is multiplied by DOC concentration in each computational cell to leave a value that has units of per meter, which is the same as standard extinction coefficients and therefore is able to be added to other (e.g. background) parallel extinction coefficients

Settling

Navigation row for this command. Argument syntax depends on the selected implementation. Refer to the implementation specific sections immediately below.

Settling == V_{settle}^{FRP}

Model Construction: Section [4.7.3.4.2](#)

Used in an inorganic phosphorus constituent model block to control the settling rate of adsorbed FRP. This will be linked directly to the TUFLOW FV ST Module in future releases of the WQ Module.

V_{settle}^{FRP} - Constant Rate of Adsorbed FRP Settling

Default: 0

Units: m/d

Range: (-50, 0)

Science: Section [F.5](#)

The constant settling velocity applied to adsorbed FRP. Future releases of the WQ Module will dynamically link this settling velocity to calculations made by the TUFLOW FV ST Module. A negative value is a downwards velocity

Settling == V_{settle}^{pth}

Model Construction: Section [4.6.3.2.1](#)

Used in an (optional) pathogens constituent model block to set free pathogen settling velocities. This will be linked directly to the TUFLOW FV ST Module in future releases of the WQ Module.

V_{settle}^{pth} - Unattached Pathogen Settling Velocity

Default: 0

Units: m/d

Range: (-50, 0)

Science: Section [N.4](#)

The settling velocity of unattached pathogens. A negative value is a downwards velocity. Future releases of the WQ Module will dynamically link settling velocity to calculations made by the TUFLOW FV ST Module

Settling == $V_{settle}^{pth}, V_{settle}^{pth_t}$

Model Construction: Section [4.6.3.2.2](#)

Used in an (optional) pathogens constituent model block to set free and attached pathogen settling velocities. This will be linked directly to the TUFLOW FV ST Module in future releases of the WQ Module.

V_{settle}^{pth} - Unattached Pathogen Settling Velocity

Default: 0

Units: m/d

Range: (-50, 0)

Science: Section [N.4](#)

The settling velocity of unattached pathogens. A negative value is a downwards velocity. Future releases of the WQ Module will dynamically link settling velocity to calculations made by the TUFLOW FV ST Module

$V_{settle}^{pth_t}$ - Attached Pathogen Settling Velocity

Default: 0

Units: m/d

Range: (-50, 0)

Science: Section [N.4](#)

The settling velocity of attached pathogens. A negative value is a downwards velocity. Future releases of the WQ Module will dynamically link settling velocity to calculations made by the TUFLOW FV ST Module

Settling == Constant, V_{settle}^{long}

Model Construction: Section [4.8.3.5.1](#)

Used in an organic matter constituent model block to control the settling rate of labile particulate organic matter. This will be linked directly to the TUFLOW FV ST Module in future releases of the WQ Module.

For further information on the constant organic settling model, refer to Section [M.8.2](#).

V_{settle}^{lorg} - Labile Organic Matter Settling Velocity

Default: 0

Units: m/d

Range: (-50, 0)

Science: Section [M.8.2](#)

The settling velocity applied to labile particulate organic matter for constant or density related settling calculations. A negative value is a downwards velocity. Future releases of the WQ Module will dynamically link settling velocity to calculations made by the TUFLOW FV ST Module

Settling == Constant, V_{settle}^{phy}

Model Construction: Section [4.7.3.5.1.12](#)

Used in a phytoplankton constituent model block to set a constant settling velocity in both basic and advanced phytoplankton constituent models. A negative value specified in this command is a downwards velocity. Setting the settling velocity to zero in this model is the same as setting **Settling** to None.

For further information on the constant phytoplankton settling model, refer to Section [H.4.2](#).

V_{settle}^{phy} - Constant Rate of Phytoplankton Settling

Default: 0

Units: m/d

Range: (-50, 0)

Science: Section [H.4.2](#)

The constant settling velocity applied to phytoplankton using either the basic or advanced phytoplankton constituent model. It is applied as a constant (in the constant settling model) or modified by density (using the density correction model). A negative value is a downwards velocity

Settling == Motile, V_{mot}^{phy} , I_{K-mot}

Model Construction: Section [4.7.3.5.2.4](#)

Used in a phytoplankton constituent model block to compute settling velocity via motility functions that depend on ambient conditions, in only the advanced phytoplankton constituent model. The specification of I_K is not mandatory in this command. If it is not specified then the I_K specified in the phytoplankton constituent model's light limitation model will be used. If a light limitation model is not specified, or uses I_S instead of I_K , then the library default value of I_K is used. If I_K is specified both in this motile settling command and a phytoplankton constituent model light limitation function, then the value specified in the [Light Limitation](#) command is used, and the value specified in this command is ignored.

For further information on the motile phytoplankton settling model, refer to Section [H.4.5](#).

V_{mot}^{phy} - Motile Settling Velocity

Default: 0

Units: m/d

Range: (-50, 0)

Science: Section [H.4.5](#)

The motile settling velocity applied to phytoplankton, that is then modified by local light conditions. It can be applied to only to the advanced phytoplankton constituent model. A negative value is a downwards velocity

I_{K-mot} - Motile Settling Light Half Saturation Light Intensity

Default: 20

Units: W/m²

Range: (0, 1500)

Science: Section [H.4.5](#)

The half saturation light intensity used to compute direction of motility. It can be applied only to the advanced phytoplankton constituent model. This value is ignored if I_K has been specified in a light limitation model within the same phytoplankton constituent model block

Settling == None

Model Construction: Section [4.8.3.5.1](#)

Used in an organic matter constituent model block to set the settling rate of labile particulate organic matter to zero.

For further information on the science of this command, refer to Section [M.8.1](#).

Settling == None

Model Construction: Section [4.7.3.5.1.12](#)

Used in a phytoplankton constituent model block to turn off settling in both basic and advanced phytoplankton constituent models.

For more information on the science of this command, refer to Section [H.4.1](#).

Settling == Stokes, d_{lorg} , ρ_{lorg}

Model Construction: Section [4.8.3.5.1](#)

Used in an organic matter constituent model block to control the settling rate of labile particulate organic matter. This will be linked directly to the TUFLOW FV ST Module in future releases of the WQ Module.

For further information on the stokes organic settling model, refer to Section [M.8.4](#).

d_{lorg} - Labile Organic Matter Stokes Diameter

Default: 1 e-09

Units: m

Range: (1 e-09, 1 e -06)

Science: Section [M.8.4](#)

The conceptual diameter of labile particulate organic matter applied in stokes calculations of settling velocity. Future releases of the WQ Module will dynamically link settling velocity to calculations made by the TUFLOW FV ST Module

ρ_{lorg} - Labile Organic Matter Stokes Density

Default: 2000

Units: kg/m³

Range: (1000, 3000)

Science: Section [M.8.4](#)

The density of labile particulate organic matter applied in stokes calculations of settling velocity. Future releases of the WQ Module will dynamically link settling velocity to calculations made by the TUFLOW FV ST Module

Settling == Stokes, I_{K-sto}

Model Construction: Section [4.7.3.5.1.12](#)

Used in a phytoplankton constituent model block to compute settling velocity via stokes settling laws in both basic and advanced phytoplankton constituent models. Density must be simulated as a computed variable for each phytoplankton group that uses this model, so must have cell density initial conditions and boundary conditions specified as per ordering rules. The specification of I_K is not mandatory in this command. If it is not specified then the I_K specified in the phytoplankton constituent model's light limitation model will be used. If a light limitation model is not specified, or uses I_S instead of I_K , then the library default value of I_K is used. If I_K is specified both in this stokes settling command and a phytoplankton constituent model light limitation function, then the value specified in the **Light Limitation** command is used, and the value specified in this command is ignored.

For further information on the stokes phytoplankton settling model, refer to Section [H.4.4](#).

I_{K-sto} - Stokes Settling Light Half Saturation Light Intensity

Default: 20

Units: W/m²

Range: (0, 1500)

Science: Section [H.4.4](#)

The half saturation light intensity used to compute cell density, which is in turn required for calculation of Stokes settling velocity. It can be applied to either the basic or advanced phytoplankton constituent model. This value is ignored if I_K has been specified in a light limitation model within the same phytoplankton constituent model block

Settling == Thermal, V_{settle}^{org}

Model Construction: Section [4.8.3.5.1](#)

Used in an organic matter constituent model block to control the settling rate of labile particulate organic matter. This will be linked directly to the TUFLOW FV ST Module in future releases of the WQ Module.

For further information on the thermal organic settling model, refer to Section [M.8.3](#).

V_{settle}^{org} - Labile Organic Matter Settling velocity

Default: 0

Units: m/d

Range: (-50, 0)

Science: Section [M.8.2](#)

The settling velocity applied to labile particulate organic matter for constant or density related settling calculations. A negative value is a downwards velocity. Future releases of the WQ Module will dynamically link settling velocity to calculations made by the TUFLOW FV ST Module

Settling == Thermal, V_{settle}^{phy}

Model Construction: Section [4.7.3.5.1.12](#)

Used in a phytoplankton constituent model block to set a constant settling velocity in both basic and advanced phytoplankton constituent models, allowing for temperature effects to settling. A negative value specified in this command is a downwards velocity.

For further information on the thermal phytoplankton settling model, refer to Section [H.4.3](#).

V_{settle}^{phy} - Constant Rate of Phytoplankton Settling

Default: 0

Units: m/d

Range: (-50, 0)

Science: Section [H.4.2](#)

The constant settling velocity applied to phytoplankton using either the basic or advanced phytoplankton constituent model. It is applied as a constant (in the constant settling model) or modified by density (using the density correction model). A negative value is a downwards velocity

Silicate Benthic == $K_{sed-O_2}^{Si}$, θ_{sed}^{Si}

Model Construction: Section [4.7.3.2.1](#)

Used in a silicate constituent model block to control the response of benthic silicate flux to temperature and oxygen concentration.

$K_{sed-O_2}^{Si}$ - Sediment Half Saturation Oxygen Concentration for Silicate Flux

Units	Range	Default
mg/L O ₂	(0, 4.8)	4
mmol/m ³ O ₂	(0, 150)	125

Science: Section [D.1](#)

The dissolved oxygen concentration for which the computed sediment silicate flux is half the user specified rate, at 20°C. Cannot be varied spatially

θ_{sed}^{Si} - Sediment Silicate Flux Temperature Coefficient

Default: 1

Units: NA

Range: (1, 1.1)

Science: Section [D.1](#)

The factor to which (T-20) is raised to account for temperature effects on silicate sediment flux. A value of 1.0 will remove the effect of temperature

Silicate Flux == F_{sed}^{Si}

Model Construction: Section [4.7.4](#)

Used in a materials block to control the sediment flux rate of silicate.

F_{sed}^{Si} - Sediment Silicate Flux

Units	Range	Default
mg Si/m ² /d	(0, 140)	0
mmol Si/m ² /d	(0, 5)	0

Science: Section [D.1](#)

The rate at which silicate is exchanged between the sediments and overlying water column at 20°C excluding the influence of overlying dissolved oxygen concentration. Can be varied spatially via use of model mesh material types. This is not the maximum rate of silicate sediment flux.

This parameter is output as a diagnostic variable. For further information, refer to [Silicate User Defined Sediment Flux](#).

silicate Limitation == $[Si]_{min}^{phy}$, K_{lim-Si}^{phy}

Model Construction: Section 4.7.3.5.1.6

Used in a phytoplankton constituent model block to set silicate limitation parameters for the basic phytoplankton model. Specifying this command triggers silicate uptake.

$[Si]_{min}^{phy}$ - Minimum Concentration of Silicate for Phytoplankton Uptake

Units	Range	Default
mg/L Si	(0, 0.1)	0.01
mmol/m ³ Si	(0.00, 3.57)	0.36

Science: Section I.5

Used to compute the silicate limitation function in the basic and advanced phytoplankton model. It is the minimum silicate concentration at which uptake of silicate by phytoplankton can occur

K_{lim-Si}^{phy} - Half Saturation Silicate Concentration for Phytoplankton Uptake of silicate

Units	Range	Default
mg/L Si	(1, 10)	1
mmol/m ³ Si	(35.71, 357.14)	35.71

Science: Section I.5

Used to compute the silicate limitation function in the basic and advanced phytoplankton model. It is the concentration of silicate that when added to the specified minimum $[Si]_{min}^{phy}$ sets the silicate limitation function to a value of 0.5. A value of zero for this parameter will set the silicate limitation function to always be 1

silicate Min Max == $[Si]_{min}^{Si}$, $[Si]_{max}^{Si}$

Model Construction: Section 4.7.3.2.1

Used in a silicate constituent model block to set minimum and maximum silicate concentrations.

$[Si]_{min}^{Si}$ - Minimum Silicate Concentration

Units	Range	Default
mg/L Si	(0, 2.8)	NA
mmol/m ³ Si	(0, 100)	NA

Science: Appendix D

The minimum allowable silicate concentration. If the WQ Module detects a concentration less than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues. A value other than zero for this parameter would be unusual

$[Si]_{max}^{Si}$ - Maximum Silicate Concentration

Units	Range	Default
mg/L Si	(0, 140)	NA
mmol/m ³ Si	(0, 5000)	NA

Science: Appendix D

The maximum allowable silicate concentration. If the WQ Module detects a concentration greater than this, then it will be reset to this value, and reported in the WQ Module log file. The root cause for requiring this reset should be addressed as this resetting is not intended to be a permanent solution and will cause mass conservation issues

Silicate Model == Si

Model Construction: Section 4.7.3.2, sec-ConModSiSi-4

Used to commence a silicate constituent model block via specification of a constituent model from the silicate constituent model class.

Simulation Class == DO | Inorganics | Organics

Model Construction: Section 4.5.1

Used in Part 1: Simulation controls of WQ Module control file to specify water quality simulation class. If not specified, "DO" is assumed and all associated "DO" class default parameters are applied.

For further information on each simulation class, refer to Section 3.1 (DO), Section 3.2 (Inorganics) and Section 3.3 (Organics).

Target Attached Fraction == f_{att}^{pth}

Model Construction: Section 4.6.3.2.2

Used in an (optional) pathogens constituent model block to set the target attached pathogen fraction.

f_{att}^{pth} - Target Pathogen Attachment Fraction

Default: 0

Units: NA

Range: (0, 1)

Science: Section N.3

The target fraction of attached pathogens. It is computed as the concentration of attached pathogens, divided by the sum of attached and alive pathogens for each computational.

Temperature Limitation

Navigation row for this command. Argument syntax depends on the selected implementation. Refer to the implementation specific sections immediately below.

Temperature Limitation == None

Model Construction: Section 4.7.3.5.1.1

Used in a phytoplankton constituent model block to turn off phytoplankton group temperature limitation.

For further information on the science of this command, refer to Section I.2.1.

Temperature Limitation == T_{std}^{phy} , T_{opt}^{phy} , T_{max}^{phy}

Model Construction: Section 4.7.3.5.1.1

Used in a phytoplankton constituent model block to set the standard phytoplankton group temperature limitation function.

For further information on the standard temperature limitation model, refer to Section 1.2.2.

T_{std}^{phy} - Standard Temperature

Default: 10

Units: °C

Range: (5, 25)

Science: Section 1.2.2

Used to compute shape of temperature limitation function between T_{std} and T_{max} . Below T_{std} , the phytoplankton temperature limitation function is a simple Arrhenius relationship. Must always be less than the specified T_{max}

T_{opt}^{phy} - Optimum Temperature

Default: 20

Units: °C

Range: (5, 25)

Science: Section 1.2.2

Used to compute shape of temperature limitation function between T_{std} and T_{max} . Must always be less than the specified T_{max}

T_{max}^{phy} - Maximum Temperature

Default: 30

Units: °C

Range: (25, 35)

Science: Section 1.2.2

Used to compute shape of temperature limitation function between T_{std} and T_{max} . Above T_{max} , the phytoplankton temperature limitation function is 0. Must always be greater than the specified T_{std} and T_{opt}

Uptake

Navigation row for this command. Argument syntax depends on the selected implementation. Refer to the implementation specific sections immediately below.

Uptake == $R_{N-uptake}^{phy}$, $R_{P-uptake}^{phy}$, $X_{Si-C-con}^{phy}$

Model Construction: Section 4.7.3.5.2.3

Used in a phytoplankton constituent model block to set nitrogen and phosphorus (and optionally silicate) uptake rates for the advanced phytoplankton constituent model only. The silicate internal concentration ratio is ignored if silicate uptake is not activated.

$R_{N-uptake}^{phy}$ - Rate of Inorganic Nitrogen Uptake By Phytoplankton

Units	Range	Default
mg N/mg Chl <i>a</i> /d	(0.080, 2.704)	0
mmol N/mmol C/d	(0.0025, 0.086)	0

Science: Section [J.2.2](#)

Used to compute the uptake of nitrogen during growth in the advanced phytoplankton constituent model only. It is the nitrogen uptake rate per unit of phytoplankton (per day) without any influence of temperature or nutrient limitation. The unit of phytoplankton is either mg (not μg) Chl *a* or mmol C, depending on the units system used

$R_{P-uptake}^{phy}$ - Rate of Inorganic Phosphorus Uptake By Phytoplankton

Units	Range	Default
mg P/mg Chl <i>a</i> /d	(0.011, 0.374)	0
mmol P/mmol C/d	(0.0002, 0.005)	0

Science: Section [J.3.2](#)

Used to compute the uptake of phosphorus during growth in the advanced phytoplankton constituent model only. It is the phosphorus uptake rate per unit of phytoplankton (per day) without any influence of temperature or nutrient limitation. The unit of phytoplankton is either mg (not μg) Chl *a* or mmol C, depending on the units system used

$X_{Si-C-con}^{phy}$ - Constant Ratio of Internal Phytoplankton Silicate to Biomass

Units	Range	Default
mg Si/mg Chl <i>a</i>	(5.94, 11.89)	8.92
mmol Si/mmol C	(0.09, 0.19)	0.14

Science: Section [J.4](#)

Used to compute the uptake of silicate during growth in the basic and advanced phytoplankton constituent models. It should be based on the extended Redfield ratio of 106:16:1:15 or C:N:P:Si (or Chl *a* equivalent). Note the units of mg of Chl *a* rather than μg

Uptake == $X_{N-C-con}^{phy}$, $X_{P-C-con}^{phy}$, $X_{Si-C-con}^{phy}$

Model Construction: Section [4.7.3.5.1.7](#)

Used in a phytoplankton constituent model block to set constant nitrogen, phosphorus and optionally silicate to biomass ratios for the basic phytoplankton constituent model only.

$X_{N-C-con}^{phy}$ - Constant Ratio of Internal Phytoplankton N to Biomass

Units	Range	Default
mg N/mg Chl <i>a</i>	(2.97, 6.54)	4.75
mmol N/mmol C	(0.09, 0.21)	0.15

Science: Section [J.2.1](#)

Used to compute the uptake of nitrogen during growth in the basic phytoplankton constituent model only. It should be based on the Redfield ratio of 106:16:1 or C:N:P (or Chl *a* equivalent). Note the units of mg of Chl *a* rather than μg

$X_{P-C-con}^{phy}$ - Constant Ratio of Internal Phytoplankton P to Biomass

Units	Range	Default
mg P/mg Chl <i>a</i>	(0.33, 0.99)	0.66
mmol P/mmol C	(0.009, 0.014)	0.009

Science: Section [J.3.1](#)

Used to compute the uptake of phosphorus during growth in the basic phytoplankton constituent model only. It should be based on the Redfield ratio of 106:16:1 or C:N:P (or Chl *a* equivalent). Note the units of mg of Chl *a* rather than μg

$X_{Si-C-con}^{phy}$ - Constant Ratio of Internal Phytoplankton Silicate to Biomass

Units	Range	Default
mg Si/mg Chl <i>a</i>	(5.94, 11.89)	8.92
mmol Si/mmol C	(0.09, 0.19)	0.14

Science: Section [J.4](#)

Used to compute the uptake of silicate during growth in the basic and advanced phytoplankton constituent models. It should be based on the extended Redfield ratio of 106:16:1:15 or C:N:P:Si (or Chl *a* equivalent). Note the units of mg of Chl *a* rather than μg

UVA Inactivation == k_{uva}^{pth} , $c_{S_{uva}}^{pth}$, $K_{DO_{uva}}^{pth}$

Model Construction: Section [4.6.3.2.1](#)

Used in an (optional) pathogens constituent model block to control the inactivation of pathogens due to UV-A light.

k_{uva}^{pth} - Pathogen Freshwater Inactivation Rate Coefficient for Exposure to UV-A Light

Default: 0

Units: m^2/MJ

Range: (0, 20)

Science: Section [N.2](#)

Inactivation effect of UV-A radiation. Excludes the effect of salinity and oxygen on inactivation

$c_{S_{uva}}^{pth}$ - Coefficient That Enhances The Inactivation Effect of UV-A Light Under Saline Conditions

Default: 0

Units: $\text{m}^2/\text{MJ}/\text{psu}$

Range: (0, 0.007)

Science: Section [N.2](#)

Enhancement of inactivation of UV-A radiation due to salinity. A value of 0.0 will remove the effect of salinity

$K_{DO_{uva}}^{pth}$ - Half Saturation Oxygen Concentration for UV-A Light Inactivation

Units	Range	Default
mg/L O_2	(0, 8)	4
	(0, 250)	125

Units	Range	Default
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Science: Section [N.2](#)

The dissolved oxygen concentration for which the computed inactivation rate under UV-A light is half that which would occur without oxygen limitation. A value of 0.0 will remove the effect of oxygen

UVB Inactivation == k_{uvb}^{pth} , $c_{S_{uvb}}^{pth}$, $K_{DO_{uvb}}^{pth}$

Model Construction: Section [4.6.3.2.1](#)

Used in an (optional) pathogens constituent model block to control the inactivation of pathogens due to UV-B light.

k_{uvb}^{pth} - Pathogen Freshwater Inactivation Rate Coefficient for Exposure to UV-B Light

Default: 0

Units: m² /MJ

Range: (0, 100)

Science: Section [N.2](#)

Inactivation effect of UV-B radiation. Excludes the effect of salinity and oxygen on inactivation

$c_{S_{uvb}}^{pth}$ - Coefficient That Enhances The Inactivation Effect of UV-B Light Under Saline Conditions

Default: 0

Units: m² /MJ /psu

Range: (0, 0.007)

Science: Section [N.2](#)

Enhancement of inactivation of UV-B radiation due to salinity. A value of 0.0 will remove the effect of salinity

$K_{DO_{uvb}}^{pth}$ - Half Saturation Oxygen Concentration for UV-B Light Inactivation

Units	Range	Default
mg/L O ₂	(0, 8)	4
	(0, 250)	125

Science: Section [N.2](#)

The dissolved oxygen concentration for which the computed inactivation rate under UV-B light is half that which would occur without oxygen limitation. A value of 0.0 will remove the effect of oxygen

visible Inactivation == k_{vis}^{pth} , $c_{S_{vis}}^{pth}$, $K_{DO_{vis}}^{pth}$

Model Construction: Section [4.6.3.2.1](#)

Used in an (optional) pathogens constituent model block to control the inactivation of pathogens due to visible light.

k_{vis}^{pth} - Pathogen Freshwater Inactivation Rate Coefficient for Exposure to Visible Light

Default: 0

Units: m² /MJ

Range: (0, 1)

Science: Section [N.2](#)

Inactivation effect of visible radiation. Excludes the effect of salinity and oxygen on inactivation

$C_{S_{vis}}^{pth}$ - Coefficient That Enhances The Inactivation Effect of Visible Light Under Saline Conditions

Default: 0

Units: m² /MJ /psu

Range: (0, 0.007)

Science: Section [N.2](#)

Enhancement of inactivation of visible radiation due to salinity. A value of 0.0 will remove the effect of salinity

$K_{DO_{vis}}^{pth}$ - Half Saturation Oxygen Concentration for Visible Light Inactivation

Units	Range	Default
mg/L O ₂	(0, 8)	4
	(0, 250)	125

Science: Section [N.2](#)

The dissolved oxygen concentration for which the computed inactivation rate under visible light is half that which would occur without oxygen limitation. A value of 0.0 will remove the effect of oxygen

water Quality Control File == water quality control file name.fvwq

Status: Required

Model Construction: Section [4.4.1](#)

Name of WQ Module control file, with no path. If this file is not in the FV control file directory, then additionally use command [water Quality Model Directory](#).

water Quality Model == TUFLOW

Status: Required

Model Construction: Section [4.4.1](#)

Instruct TUFLOW FV to activate TUFLOW WQ Module.

water Quality Model Directory == water quality control file directory

Status: Optional

Model Construction: Section [4.4.1](#)

Relative path from location of FV control file to the WQ Module control file directory, including last backslash, e.g. "..\WQM\".

wq dt == dt

Model Construction: Section [4.5.1](#)

Used in Part 1: Simulation controls of WQ Module control file to set the timestep at which TUFLOW calls the WQ Module to undertake non-conservative water quality calculations, in seconds.

dt - Timestep

Default: 900

Units: seconds

Range: (UD, UD)

The timestep at which the WQ Module is called from the hydrodynamic model

WQ Equilibrium Substeps == *f_{ess}*

Model Construction: Section [4.5.1](#)

Used in Part 1: Simulation controls of WQ Module control file to set the frequency of timesteps at which the WQ Module undertakes non-kinetic calculations, in number of water quality timesteps. This only applies to FRP adsorption.

f_{ess} - Non-Kinetic Equilibrium Substep Frequency

Default: 1

Units: Number of WQ Module timesteps

Range: (1, UD)

The frequency (in WQ timesteps) at which the WQ Module calls non-kinetic equilibrium calculations. for example, a value of 12 will call non-kinetic calculations every twelfth time the WQ module is called

WQ Units == mgL | mmm

Model Construction: Section [4.5.1](#)

Used in Part 1: Simulation controls of WQ Module control file to set the units used for water quality simulation. Milligrams per litre and millimoles per cubic metre are “mgL” and “mmm”, respectively.

For further information on units, refer to Section [4.2](#).



B Demonstration model

Explanations of the processes captured by the WQ Module are described in the Appendices that follow. A demonstration model has been constructed to generate data to support these explanations via different interactive means. This model is referred to as the demonstration model. It has the following features, unless specified otherwise:

- General
 - 1 week (168 hours) duration
 - Includes salinity, temperature (and heat calculations), sediment and varying numbers of water quality computed variables
 - Hourly output
- Geometry
 - Single two-dimensional flat bottomed cell
 - Lateral cell dimensions of 1 metre $\times$ 1 metre
 - Depth of 0.5 metres
- Boundary conditions
 - No inflows, outflows or other flow boundaries
 - Meteorological boundaries applied
 - * Hourly timestep
 - * Corresponding twenty four row record repeated for each day
 - * Wind turned off, unless noted otherwise
 - * Constant air temperature, varied to match simulation needs
 - * Typical shortwave, longwave radiation and relative humidity
- Initial conditions
 - Varied to match simulation needs
- Water quality parameterisation
 - Varied to match simulation needs

Additional model details are described in each Appendix where required.



C Processes: oxygen

C.1 Atmospheric oxygen flux

Atmospheric oxygen flux is a key source of water column dissolved oxygen. Oxygenation is implemented in the upper model layer by the WQ Module, and then this oxygenated water is mixed downwards by TUFLOW in subsequent timesteps.

Initially, a Schmidt number $Sc_{atm}^{O_2}$ is computed via Equation C.1.

$$Sc_{atm}^{O_2} = \left(0.9 + \frac{S}{350.0}\right) \times (2073.1 - 125.62T + 3.6276T^2 - 0.043219T^3) \quad (C.1)$$

T and S are ambient water temperature and salinity respectively. An oxygen piston velocity $V_{pist}^{O_2}$ (also known as a gas transfer velocity) is then computed. Two piston models for $V_{pist}^{O_2}$ are available. The first is due to Wanninkhof (1992):

$$V_{pist}^{O_2} = 0.31 \left(V_{wind}^{O_2}\right)^2 \times \left(\frac{660.0}{Sc_{atm}^{O_2}}\right)^x \quad (C.2)$$

where $V_{wind}^{O_2}$ is wind speed. For wind speed $V_{wind}^{O_2} < 3.0$ m/s, x is 0.66, otherwise x is 0.5. Wind speed is assumed to be provided from TUFLOW at 10 metres from the water surface. The second is due to Ho et al. (2016):

$$V_{pist}^{O_2} = \left(0.77 \sqrt{\frac{V_{water}}{H_{layer}}} + 0.266 \left(V_{wind}^{O_2}\right)^2\right) \times \sqrt{\frac{660.0}{Sc_{atm}^{O_2}}} \quad (C.3)$$

where V_{water} is surface water speed, H_{layer} is the thickness of the uppermost TUFLOW FV computational layer and $V_{wind}^{O_2}$ is wind speed.

There are other models available for computing both $Sc_{atm}^{O_2}$ and $V_{pist}^{O_2}$ within the WQ Module. Contact support@tuflow.com if these are required.

Once $Sc_{atm}^{O_2}$ and $V_{pist}^{O_2}$ are known, oxygenation to the surface layer is computed as per Equation C.4.

$$F_{atm}^{O_2} = V_{pist}^{O_2} ([DO]_{air} - [DO]) \quad (C.4)$$

$F_{atm}^{O_2}$ is the flux of atmospheric oxygen to the surface layer, and $[DO]_{air}$ and $[DO]$ are the oxygen concentrations in air and water (as a computed variable in a computational cell) at the air-water interface, respectively. $[DO]_{air}$ is assumed to be the saturation concentration of dissolved oxygen in water which is at the ambient surface water's temperature and salinity conditions. As such, supersaturated surface waters will release dissolved oxygen to the atmosphere under this schematisation. Oxygen percent saturation is computed as per Equation C.5.

$$\left. \begin{aligned}
[DO]_{psat} &= 100.0 \times \frac{[DO]}{[DO]_{sat}} \\
[DO]_{sat} &= 1.42763 \times e^C \\
C &= -173.4292 + \left(249.6339 \times \frac{100.0}{T + 273.15} \right) + \left(143.3483 \times \ln \left(\frac{T + 273.15}{100.0} \right) \right) \dots \\
&\quad \left(-21.8492 \times \frac{T + 273.15}{100.0} \right) \dots \\
&\quad - S \times \left(-0.033096 + \left(0.014259 \times \frac{T + 273.15}{100.0} \right) - 0.0017 \times \left(\frac{T + 273.15}{100.0} \right)^{2.0} \right)
\end{aligned} \right\} \quad (C.5)$$

T and S are ambient water temperature and salinity respectively.

C.2 Sediment oxygen flux

Oxygen is exchanged between the water column and sediments via specification of a sediment flux representing the net effect of biological activity. In the case of oxygen, this flux is most commonly into the sediments, i.e. a negative sediment flux. Although it is rare that sediments act as sources of oxygen, the WQ Module can be parameterised to allow for this if required.

The user specified sediment oxygen flux (which can be spatially varying) is modified by overlying ambient dissolved oxygen concentration (together with a user specified half saturation oxygen concentration) and water temperature. These modifications are simulated via Michaelis-Menten and Arrhenius models, respectively, as per Equation C.6.

$$F_{sed}^{O_2}(\text{computed}) = F_{sed}^{O_2} \times \underbrace{\frac{[DO]}{K_{sed-O_2}^{O_2} + [DO]}}_{\text{Influence of oxygen}} \times \underbrace{[\theta_{sed}^{O_2}]^{(T-20)}}_{\text{Influence of temperature}} \quad (C.6)$$

$F_{sed}^{O_2}$ is the user specified oxygen sediment flux at 20°C without the influence of dissolved oxygen, $[DO]$ is the overlying dissolved oxygen concentration computed by the WQ Module, $K_{sed-O_2}^{O_2}$ and $\theta_{sed}^{O_2}$ are the half saturation oxygen concentration and temperature coefficient for dissolved oxygen sediment flux respectively, and T is ambient water temperature.

The form of the above relationship between dissolved oxygen concentration and the computed oxygen sediment flux, for a range of $K_{sed-O_2}^{O_2}$ values is provided in Figure C.1. Water temperature is held constant at 20°C and $\theta_{sed}^{O_2} = 1$ (i.e. the Arrhenius temperature function is switched off). The user specified benthic oxygen sediment flux is -4,800 mg/m²/day. Use the “play” button or drag the slider to see how different half saturation oxygen concentrations change the oxygen sediment flux (ordinate), as a function of ambient dissolved oxygen concentration (abscissa).

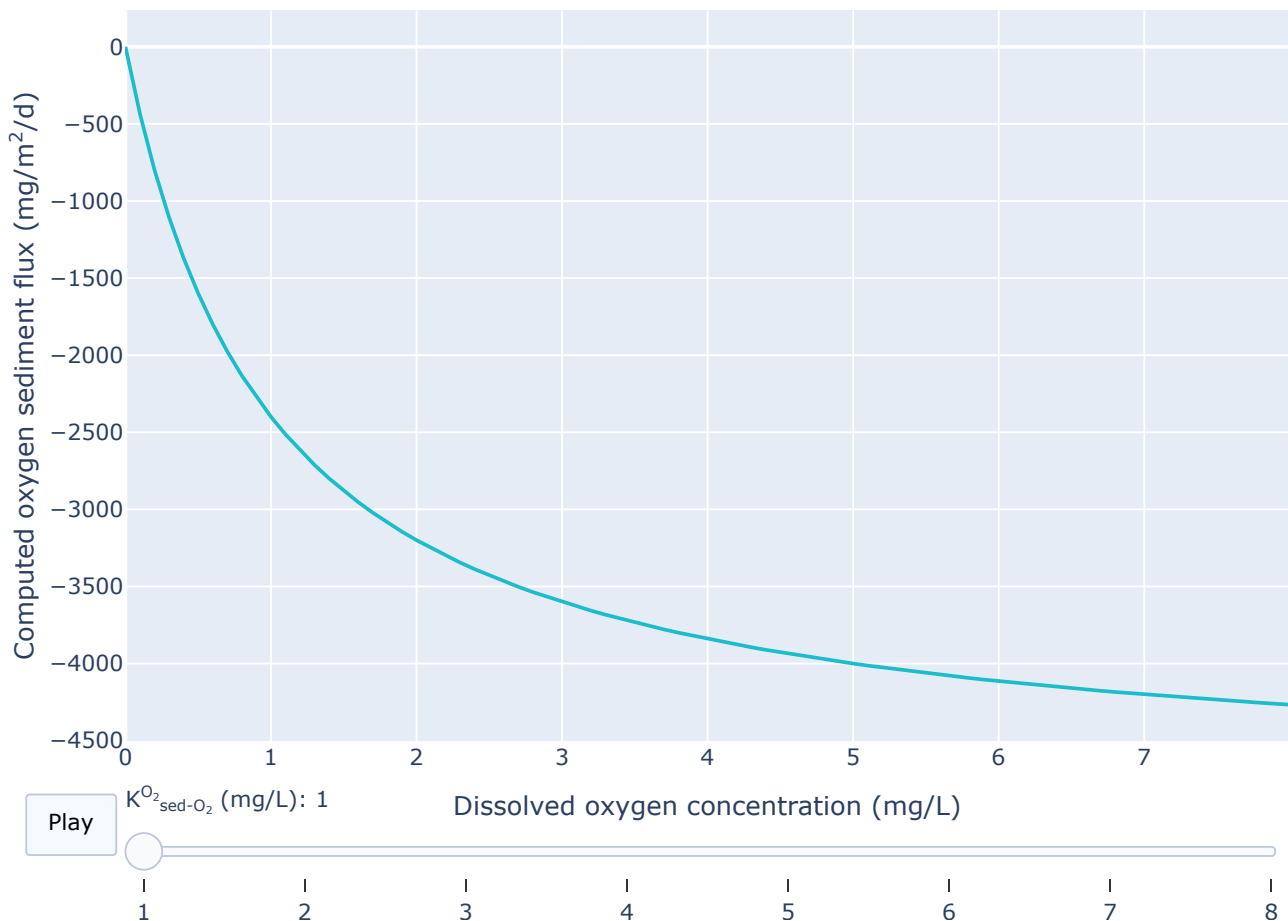


Figure C.1: Move the slider to see the effect of changing $K_{sed-O_2}^{O_2}$ on the computed oxygen sediment flux

The figure demonstrates that in this example, the smaller the value of $K_{sed-O_2}^{O_2}$, the faster the magnitude of the computed oxygen sediment flux increases with ambient dissolved oxygen concentration. This is consistent with one interpretation of $K_{sed-O_2}^{O_2}$, that it is the ambient dissolved oxygen concentration at which the computed oxygen sediment flux is half that of the user specified $F_{sed}^{O_2}$, when temperature effects are turned off.

In light of the above, the demonstration model has been used to illustrate the influence that the half saturation concentration has on the rate of drawdown of water column dissolved oxygen. The model was repeatedly executed using a different $K_{sed-O_2}^{O_2}$ for each simulation, but at the same water temperature of (approximately) 20°C, and with temperature effects turned off. The predicted temporal evolution of water column dissolved oxygen concentration is provided in Figure C.2. Use the “play” button or drag the slider to see how different half saturation oxygen concentrations change the rate of dissolved oxygen (ordinate) drawdown with time (abscissa).

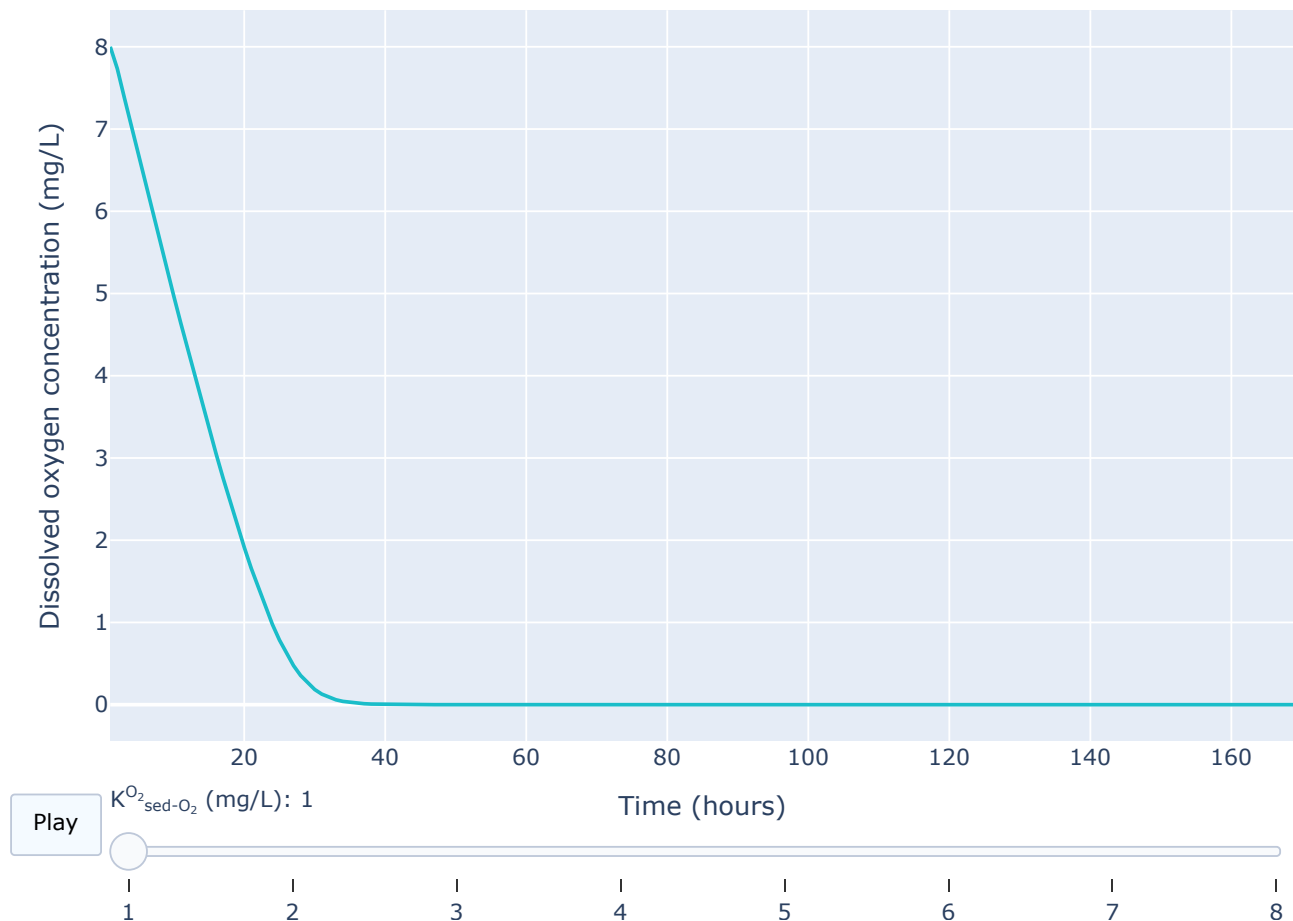


Figure C.2: Move the slider to see the effect of changing $K^{O_2}_{sed-O_2}$ on the rate of consumption of dissolved oxygen in water immediately above the sediments

Consistent with the behaviour demonstrated in Figure C.1, Figure C.2 has a less rapid drawdown of ambient dissolved oxygen concentrations with increasing $K^{O_2}_{sed-O_2}$.

The rate of dissolved oxygen drawdown is also related to ambient water temperature, via the Arrhenius model in Equation C.6. To illustrate this, the demonstration model was executed at a range of ambient temperatures, a constant half saturation oxygen concentration for oxygen sediment flux of 4 mg/L and a temperature factor $\theta^{O_2}_{sed}$ of 1.05. The results are provided in Figure C.3. Use the “play” button or drag the slider to see how different ambient temperatures change the rate of dissolved oxygen (ordinate) drawdown under these conditions, with time (abscissa).

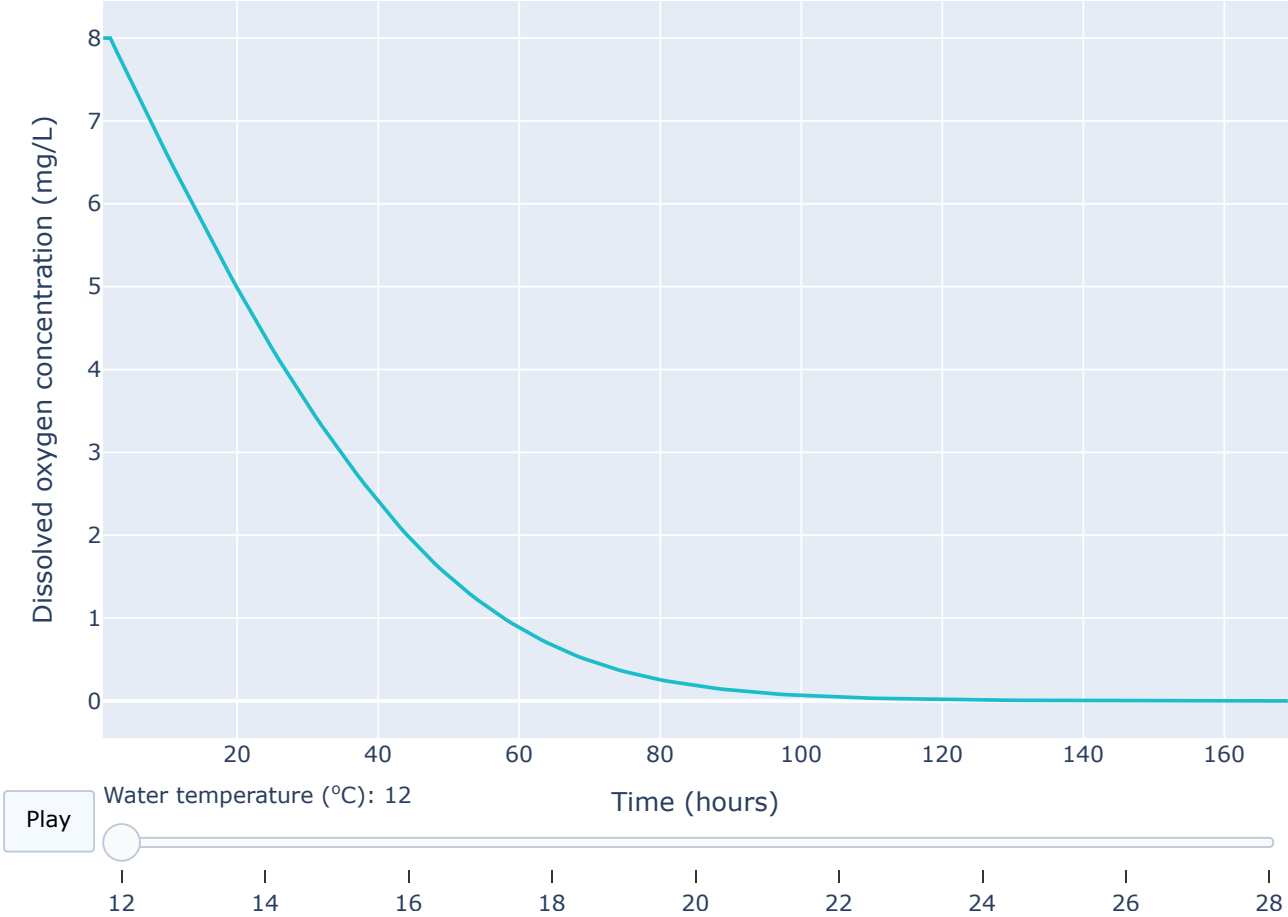


Figure C.3: Move the slider to see the effect of changing the ambient water temperature on dissolved oxygen concentrations

The figure confirms the expected result that the rate of dissolved oxygen drawdown increases with increasing ambient water temperature. This increased rate reflects the expected increase in benthic biological activity with temperature.



D Processes: silicate

D.1 Sediment silicate flux

Silicate is exchanged between the water column and sediments via specification of a sediment flux. In the case of silicate, this flux is most commonly out of the sediments, i.e. a positive specification of sediment flux. Although it is rare that sediments act as sinks of silicate, the WQ Module can be parameterised to allow for this if required.

The user specified rate of sediment silicate flux (which can be spatially varying) is modified by overlying ambient dissolved oxygen concentration, a user specified half saturation oxygen concentration and water temperature. These modifications are simulated via Michaelis-Menten and Arrhenius models, respectively, as per Equation D.1.

$$F_{sed}^{Si(computed)} = F_{sed}^{Si} \times \underbrace{\frac{K_{sed-O_2}^{Si}}{K_{sed-O_2}^{Si} + [DO]}}_{\text{Influence of oxygen}} \times \underbrace{[\theta_{sed}^{Si}]^{(T-20)}}_{\text{Influence of temperature}} \quad (D.1)$$

F_{sed}^{Si} is the user specified silicate sediment flux at 20°C without the influence of dissolved oxygen, $[DO]$ is the overlying dissolved oxygen concentration, $K_{sed-O_2}^{Si}$ and θ_{sed}^{Si} are the half saturation concentration of dissolved oxygen and temperature coefficient for silicate sediment production respectively (both are user specified), and T is ambient water temperature.

The form of the above relationship between dissolved oxygen concentration and the computed silicate sediment flux, for a range of $K_{sed-O_2}^{Si}$ values is provided in Figure D.1. Water temperature is held constant at 20°C and $\theta_{sed}^{Si}=1$ (i.e. the Arrhenius temperature function is switched off). The user specified benthic silicate sediment flux is 1,120 mg/m²/day. Use the “play” button or drag the slider to see how different half saturation oxygen concentrations change the silicate sediment flux (ordinate) with dissolved oxygen concentration (abscissa).

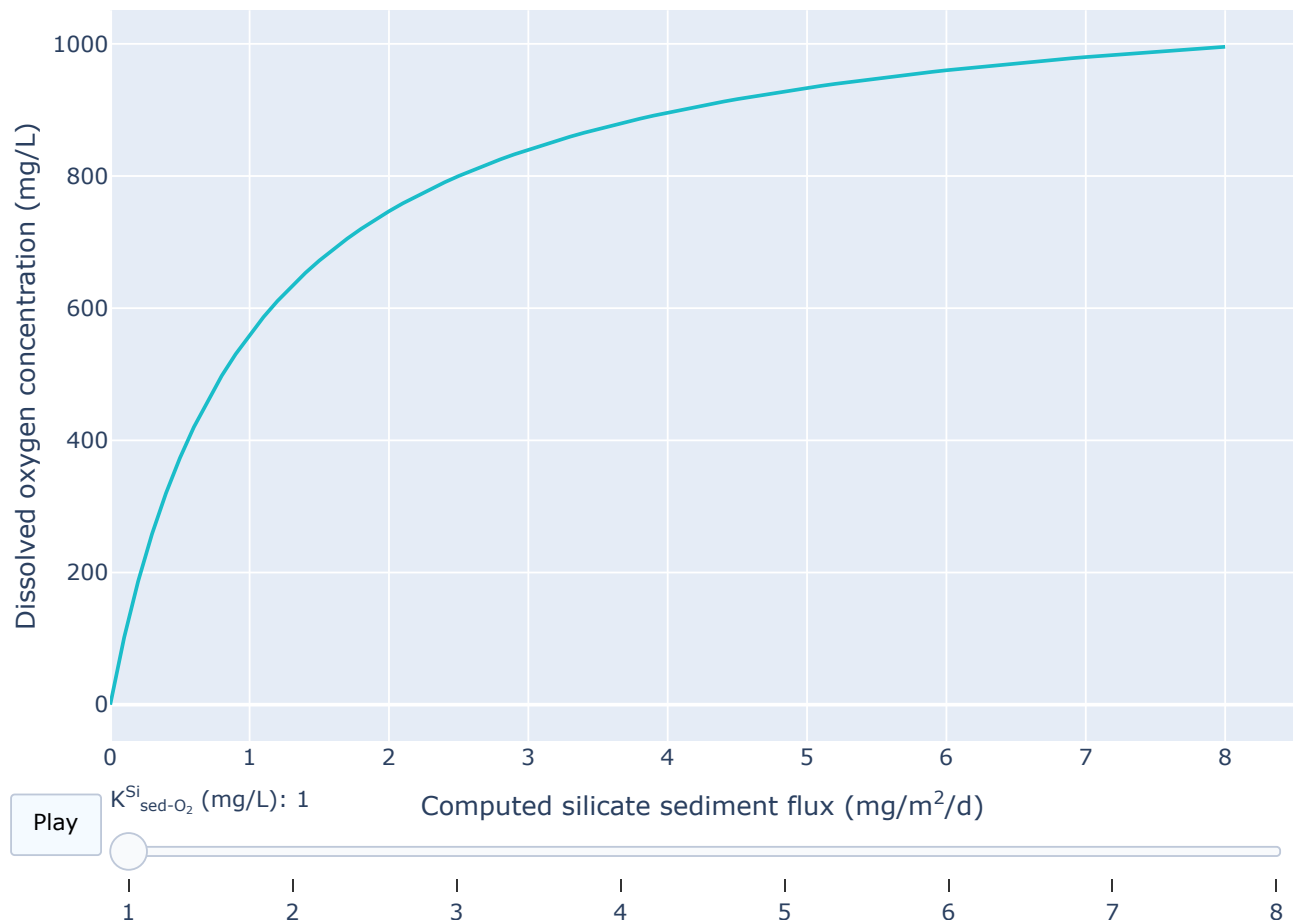


Figure D.1: Move the slider to see the effect of changing the $K_{sed-O_2}^{Si}$ value on the computed silicate sediment flux

The figure demonstrates that in this example, the smaller the value of $K_{sed-O_2}^{Si}$, the faster the magnitude of the computed silicate sediment flux increases with ambient dissolved oxygen concentration. This is consistent with one interpretation of $K_{sed-O_2}^{Si}$, that it is the ambient dissolved oxygen concentration at which the computed silicate sediment flux is half that of the user specified F_{sed}^{Si} , when temperature effects are turned off.

More generally, for constant dissolved oxygen concentration and $K_{sed-O_2}^{Si}$ and without temperature effects, Equation D.1 has that the computed silicate sediment flux is constant. This means that silicate drawdown also occurs at a constant rate in the demonstration model, so the figure analogous to Figure C.2 is not presented here.

A more realistic environmental setting has sediment silicate fluxes occurring against a background of oxygen concentration drawdown. The demonstration model has been used to illustrate this via execution of a suite of simulations that experience dissolved oxygen drawdown (in the dissolved oxygen constituent model, with $K_{sed-O_2}^{O_2} = 4$ mg/L) and each simulation using a different value of $K_{sed-O_2}^{Si}$. The silicate sediment flux rate was specified as above and temperature effects were turned off. The predicted temporal evolution of water column silicate concentration is provided in Figure D.2. Use the “play” button or drag the slider to see how different half saturation concentrations change predicted silicate concentrations (ordinate) in time (abscissa).

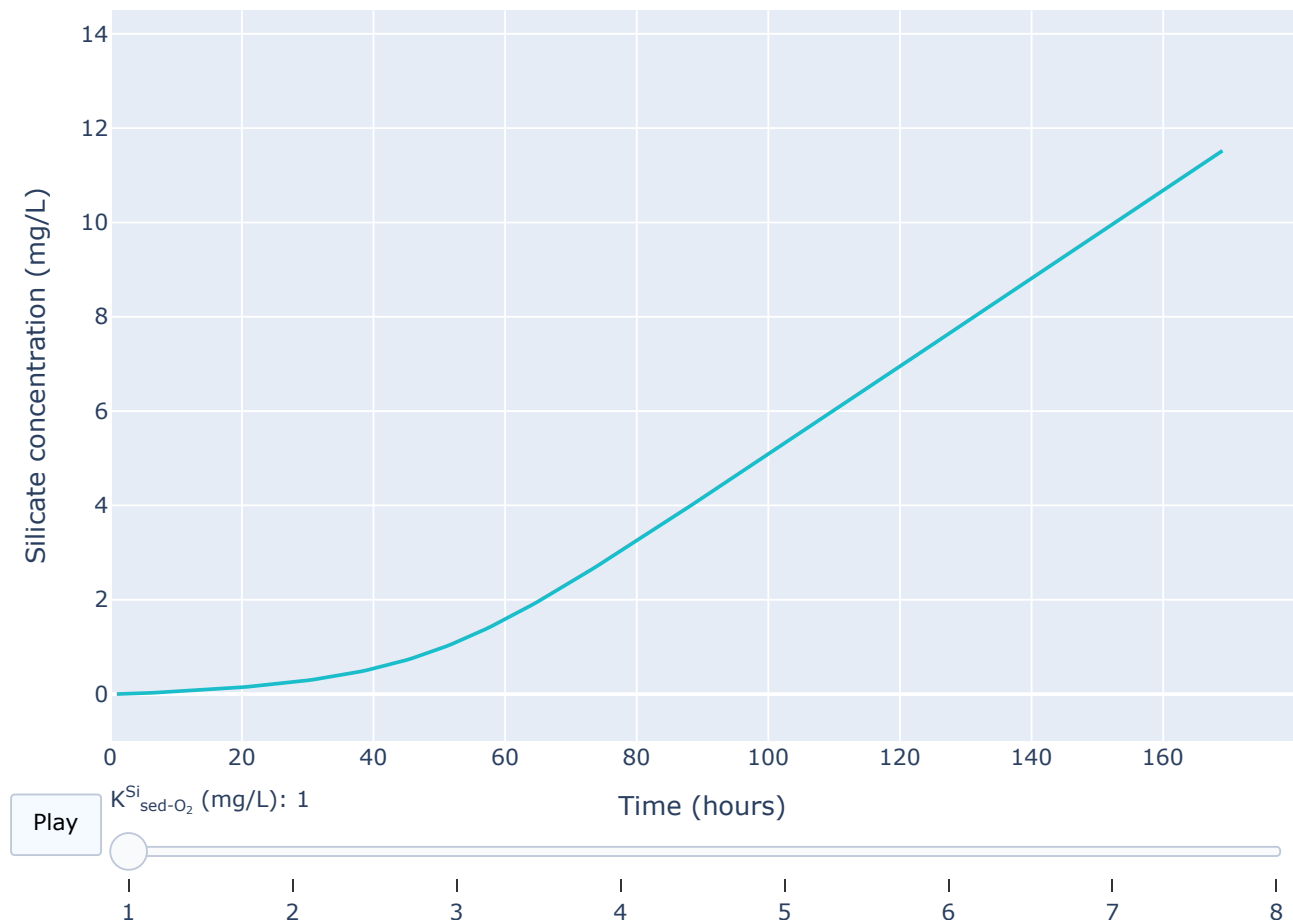


Figure D.2: Move the slider to see the effect of changing the $K_{sed-O_2}^{Si}$ value on the rate of production of silicate in water immediately above the sediments

Finally, the demonstration model was executed over a suite of simulations that had constant sediment flux rates (as above), half saturation coefficients (both $K_{sed-O_2}^{O_2}$ and $K_{sed-O_2}^{Si} = 4$ mg/L) and temperature coefficients (both $\theta_{sed}^{O_2}$ and $\theta_{sed}^{Si} = 1.05$), but varied ambient water temperature. The predicted temporal evolution of water column silicate concentration is provided in Figure D.3. Use the “play” button or drag the slider to see how different water temperatures change silicate concentrations (ordinate) in time (abscissa).

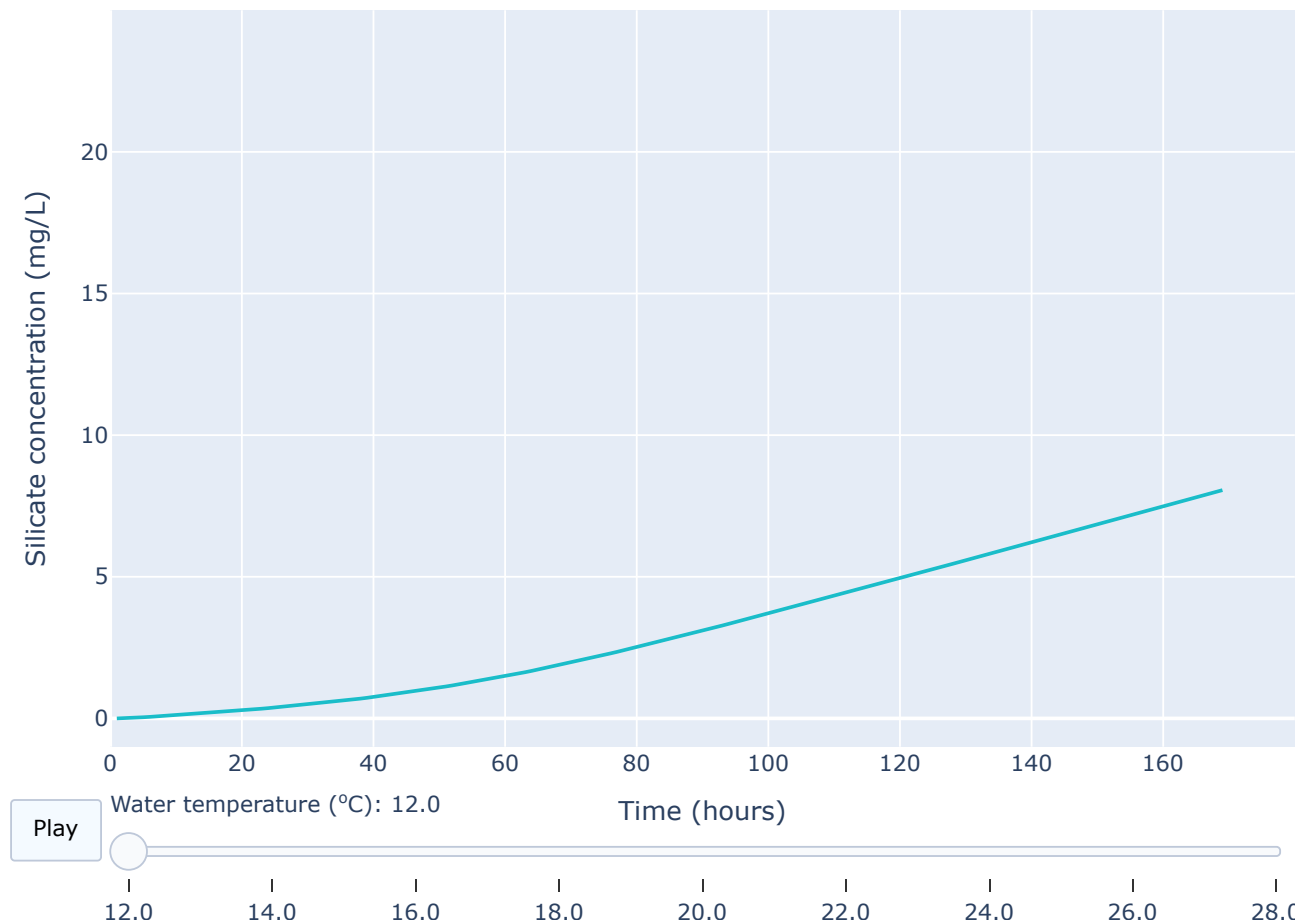


Figure D.3: Move the slider to see the effect of changing the ambient water temperature on silicate concentration

Although not recommended, the influence of oxygen in all the above processes can be removed by setting the command `oxygen == off` in the silicate model block.



E Processes: inorganic nitrogen

E.1 Sediment ammonium and nitrate flux

Ammonium and nitrate are exchanged between the water column and sediments via specification of separate sediment fluxes. In both cases, this flux is most commonly out of the sediments, i.e. a positive specification of sediment flux. Although it is rare that sediments act as sinks of these nitrogenous species, the WQ Module can be parameterised to allow for this if required.

The user specified rates of ammonium and nitrate fluxes (which can be spatially varying) are modified by overlying ambient dissolved oxygen concentration (together with respective user specified half saturation oxygen concentrations) and water temperature. These modifications are simulated via Michaelis-Menten and Arrhenius models, respectively, as per Equation E.1.

$$\left. \begin{aligned} F_{sed(computed)}^{NH_4} &= F_{sed}^{NH_4} \times \frac{K_{sed-O_2}^{NH_4}}{K_{sed-O_2}^{NH_4} + [DO]} \times \underbrace{[\theta_{sed}^{NH_4}]^{(T-20)}}_{\text{Influence of temperature}} \\ F_{sed(computed)}^{NO_3} &= F_{sed}^{NO_3} \times \underbrace{\frac{[DO]}{K_{sed-O_2}^{NO_3} + [DO]}}_{\text{Influence of oxygen}} \times \underbrace{[\theta_{sed}^{NO_3}]^{(T-20)}}_{\text{Influence of temperature}} \end{aligned} \right\} \quad (E.1)$$

$F_{sed}^{NH_4}$ and $F_{sed}^{NO_3}$ are the user specified ammonium and nitrate sediment fluxes at 20°C without the influence of dissolved oxygen, $[DO]$ is the overlying dissolved oxygen concentration, $K_{sed-O_2}^{NH_4}$ and $K_{sed-O_2}^{NO_3}$ are the user specified half saturation concentrations of dissolved oxygen for ammonium and nitrate sediment flux, $\theta_{sed}^{NH_4}$ and $\theta_{sed}^{NO_3}$ are the corresponding temperature coefficients, and T is ambient water temperature.

As per silicate sediment flux (see Section D.1), the above equations lead to linearly varying ambient ammonium and nitrate concentrations in the demonstration model when dissolved oxygen concentration, half saturation oxygen concentrations and ambient temperature are set to be constant.

A more realistic environmental setting has sediment ammonium and nitrate fluxes occurring against a background of oxygen concentration drawdown. The demonstration model has been used to illustrate this via execution of a suite of simulations that experience dissolved oxygen drawdown (in the dissolved oxygen constituent model, with $K_{sed-O_2}^{O_2} = 4$ mg/L) and each simulation using a the same value for both $K_{sed-O_2}^{NH_4}$ and $K_{sed-O_2}^{NO_3}$. The ammonium and nitrate sediment flux rates were both specified as 140 mg/m²/d, and temperature effects were turned off. The predicted temporal evolution of water column ammonium and nitrate concentrations is provided in Figure E.1. Use the “play” button or drag the slider to see how different half saturation concentrations change ambient concentrations (ordinate) in time (abscissa).

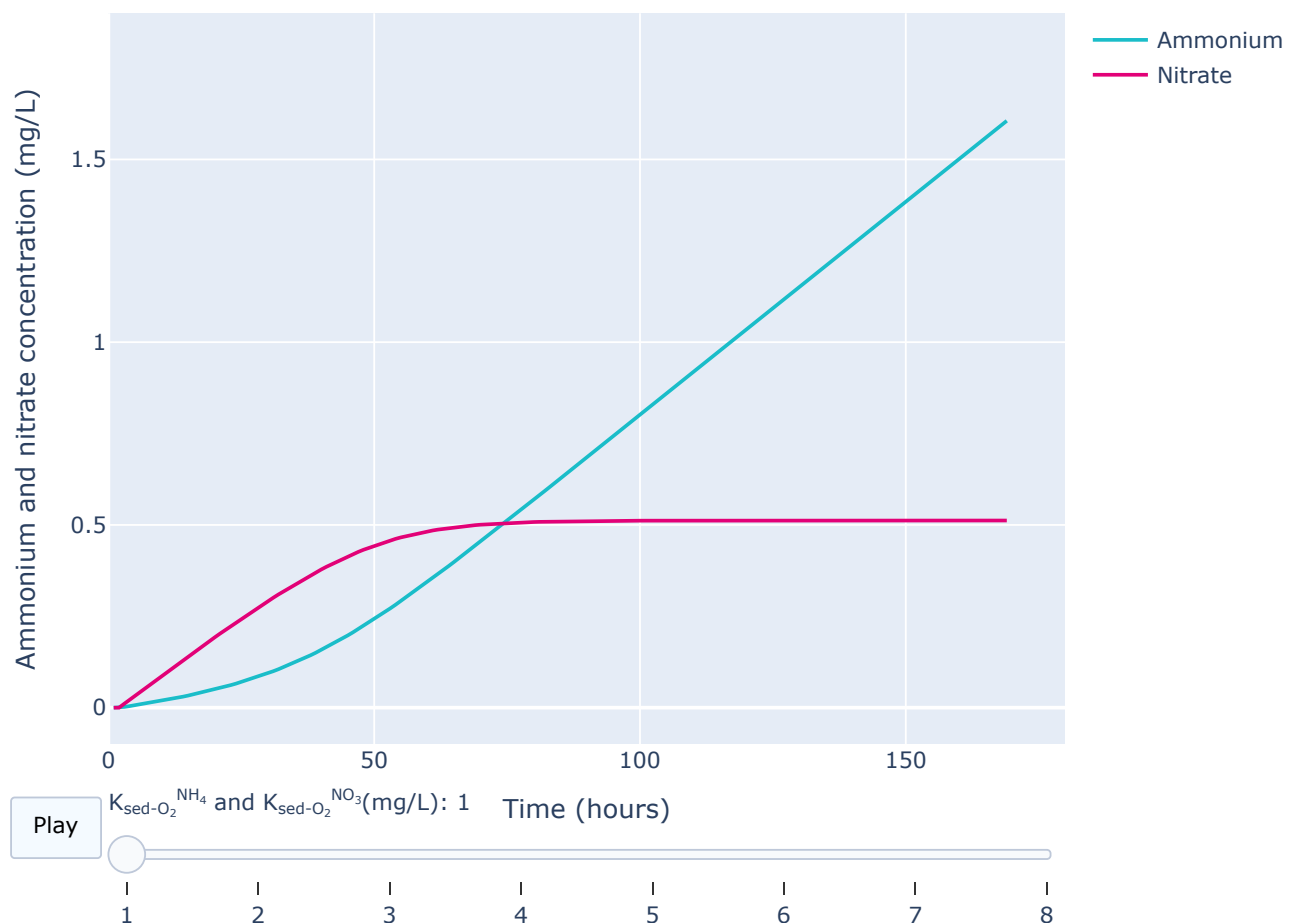


Figure E.1: Move the slider to see the effect of changing the $K_{sed-O_2}^{NH_4}$ (and $K_{sed-O_2}^{NO_3}$ - they are set to be equal to each other in this example) values on ambient ammonium and nitrate concentrations. Ambient dissolved oxygen is drawn down in time

Figure E.1 illustrates the different oxygen responses of ammonium and nitrate sediment fluxes, as reflected in the different formulations within Equation E.1. Importantly, the figure demonstrates that as ambient oxygen concentrations reach zero near 60 hours (see Figure C.2 with the slider bar set to $K_{sed-O_2}^{O_2} = 4$ mg/L), nitrate sediment flux ceases and the resultant ambient concentrations plateau. The converse is true to ammonium. One implication of this behaviour is that in environmental systems being simulated using the WQ Module, the rate of delivery of ammonium mass to the water column will generally increase under low dissolved oxygen conditions (e.g. waters isolated underneath a strong lacustrine a thermocline), whilst the corresponding nitrate mass fluxes will reduce under the same conditions. This is the expected and observed behaviour of environmental systems.

The rate of ammonium and nitrate flux is also related to ambient water temperature, via the Arrhenius model in Equation E.1. To demonstrate this, the same model above (with time varying dissolved oxygen concentration) was executed at a range of ambient temperatures, but constant half saturation concentrations for oxygen for both ammonium and nitrate set to 4 mg/L. All temperature coefficients were set to 1.05. The results are provided in Figure E.2. Use the “play” button or drag the slider to see how different ambient temperatures change the ambient ammonium and nitrate concentrations (ordinate) in time (abscissa).

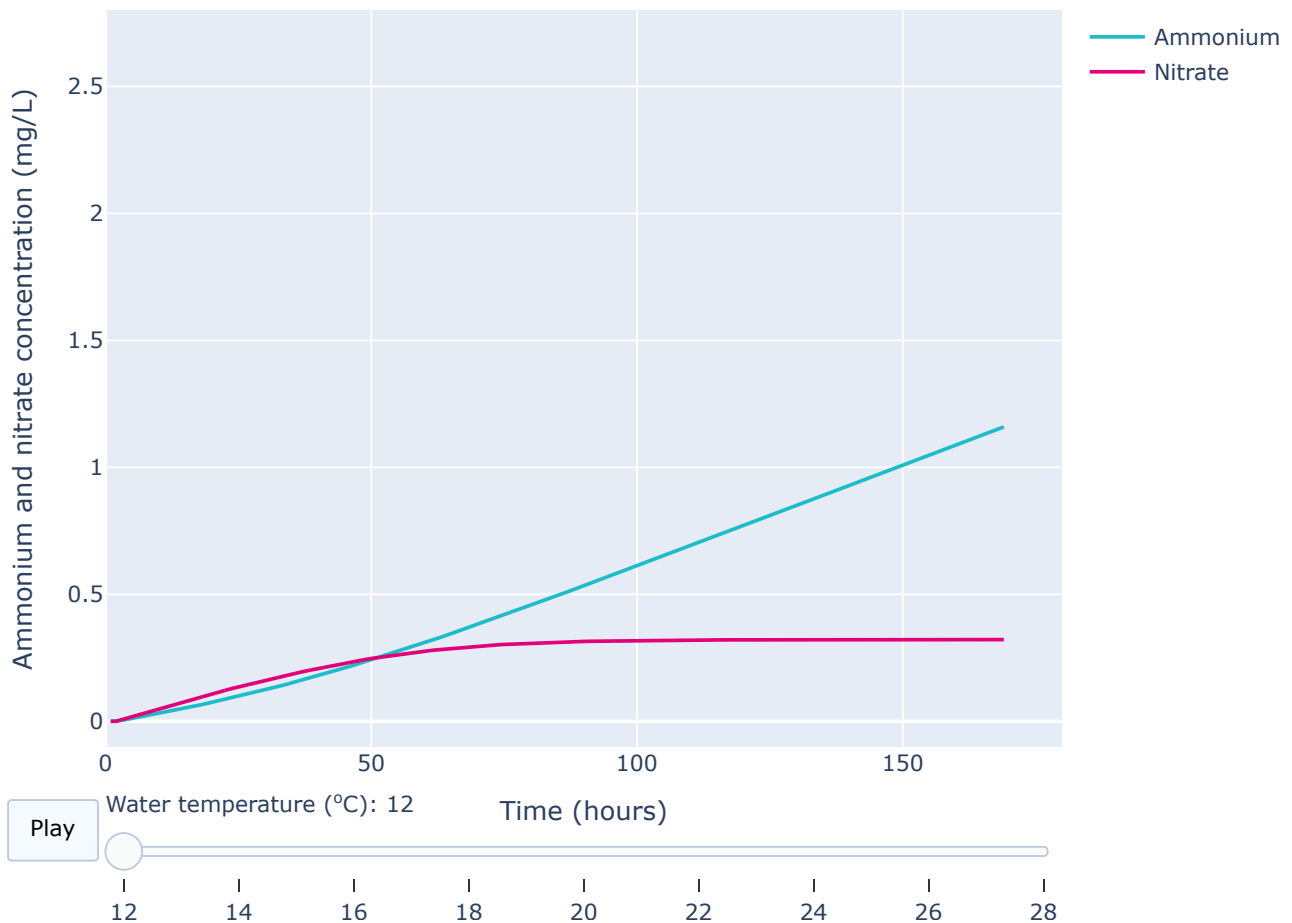
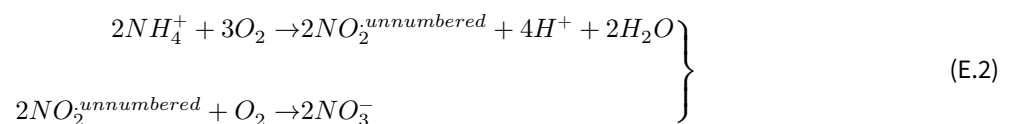


Figure E.2: Move the slider to see the effect of changing the ambient water temperature on ammonium and nitrate concentrations, with ambient dissolved oxygen drawdown

The figure shows that as ambient water temperature increases, the rate of increases of both ammonium and nitrate concentrations follow suit. Again, nitrate concentrations plateau once background dissolved oxygen concentrations reach zero, however ammonium concentrations continue to rise throughout the simulation. This is expected behaviour.

E.2 Nitrification

Nitrification is the pelagic biological oxidation of ammonium to nitrate. The equations representing this process (including intermediates) are as follows.



Dissolved oxygen is consumed by nitrification of ammonium, in a molar ratio of 1:2 N:O₂ (i.e. 2 moles of ammonium consume 4 moles of diatomic oxygen). Nitrite is an intermediate product of nitrification, and simulation of this quantity is possible within the WQ Module although not currently activated. Contact support@tufLOW.com if this capability is required.

The pelagic nitrification rate is computed within the WQ Module via Equation E.3.

$$R_{nitrif(computed)}^{NH_4} = R_{nitrif}^{NH_4} \times \underbrace{\frac{[DO]}{K_{nitrif-O_2}^{NH_4} + [DO]}}_{\text{Influence of oxygen}} \times \underbrace{\left[\theta_{nitrif}^{NH_4}\right]^{(T-20)}}_{\text{Influence of temperature}} \quad (E.3)$$

$R_{nitrif}^{NH_4}$ is the user specified ammonium nitrification rate at 20°C without the influence of dissolved oxygen, $[DO]$ is the ambient dissolved oxygen concentration, $K_{nitrif-O_2}^{NH_4}$ and $\theta_{nitrif}^{NH_4}$ are the half saturation concentration of dissolved oxygen and temperature coefficient for nitrification of ammonium respectively (both are user specified), and T is ambient water temperature.

The nitrification rate from Equation E.3 is multiplied by ambient ammonium concentration to compute the flux of ammonium to nitrate at each model timestep in each model cell via Equation E.4.

$$F_{nitrif(computed)}^{NH_4} = R_{nitrif(computed)}^{NH_4} \times [NH_4] \quad (E.4)$$

Equation E.3 reveals a linear relationship between $R_{nitrif(computed)}^{NH_4}$ and both (constant) dissolved oxygen concentration and half saturation oxygen concentration. In dissolved oxygen conditions away from oxygen sinks other than nitrification itself (such as sediments), this leaves ambient temperature as the key external determinant of the computed nitrification rates.

A suite of demonstration model simulations were executed to illustrate this, with each simulation having its own temperature, and a constant nitrification rate $R_{nitrif}^{NH_4}$ of 0.1/day. Ammonium and nitrate initial conditions were always set to 4 and 0 mg/L respectively, $K_{nitrif-O_2}^{NH_4}$ to 4 mg/L and $\theta_{nitrif}^{NH_4}$ was set to 1.05. In order to illustrate only the workings of nitrification, all sediment fluxes were set to zero. The predicted temporal evolution of water column ammonium and nitrate concentrations in these simulations are provided in Figure E.3. Corresponding dissolved oxygen concentrations are also included to demonstrate the impact of nitrification on water column oxygen. Use the “play” button or drag the slider to see how different ambient temperatures change the ambient ammonium, nitrate and dissolved oxygen concentrations (ordinate) in time (abscissa).

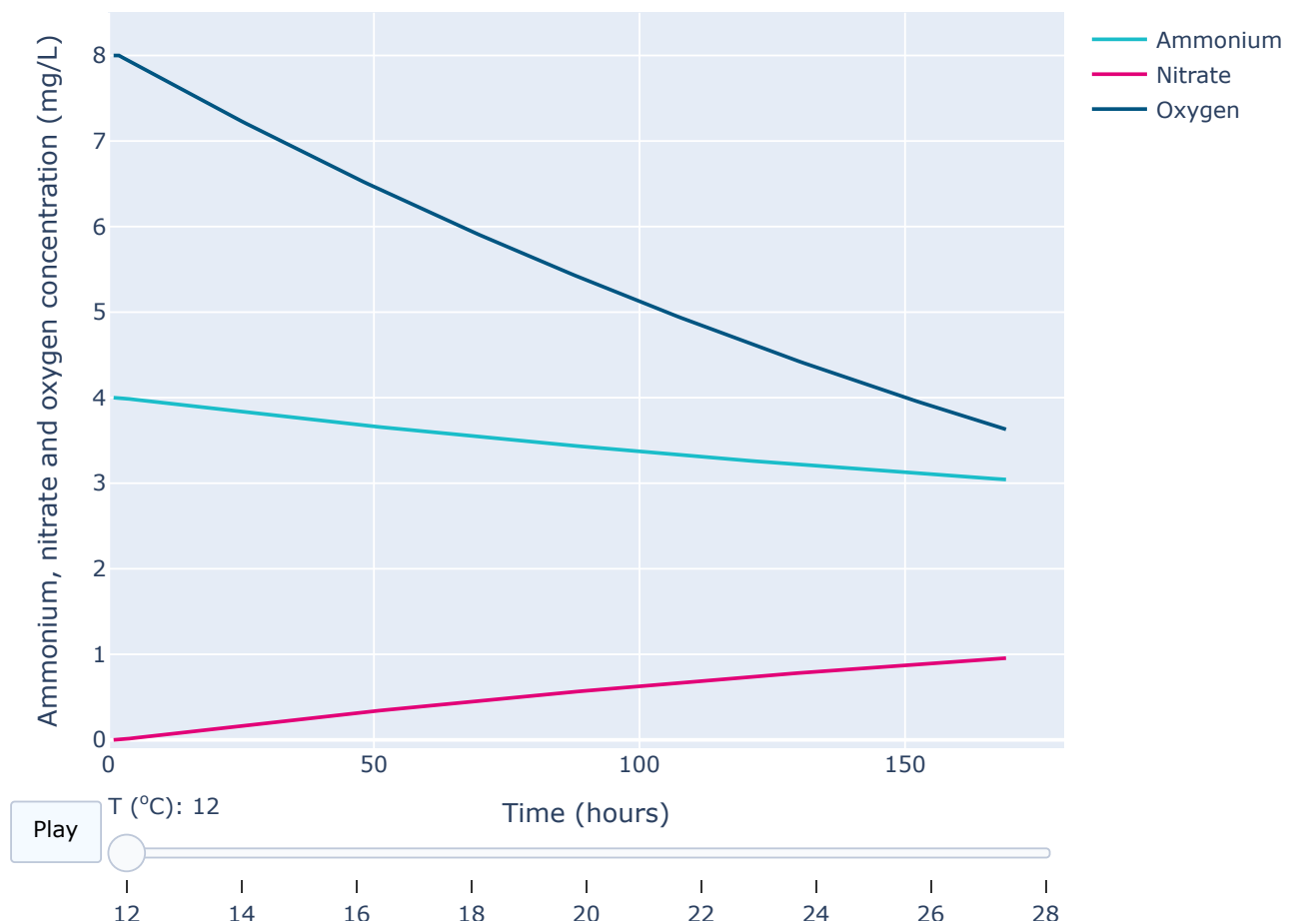


Figure E.3: Move the slider to see the effect of changing ambient water temperature on the concentrations of ammonia, nitrate and oxygen

The figure demonstrates the expected behaviour, where ammonium is consumed and nitrate produced. The drawdown

in oxygen presented in the figure is due only to nitrification.

The figure also reveals the mass conserving behaviour of the WQ Module: the decrease in ammonium (N) concentration is the same as the corresponding increase in nitrate (N) concentration for each of the different temperature simulations. This confirms the 1:1 ratio of nitrogen conversion from ammonium to nitrate in moles (Equation E.2), and hence concentration in an otherwise closed system.

The drawdown in oxygen also demonstrates the WQ Module mass balance. In the 12°C case for example:

- The change in dissolved oxygen concentration is 4.37 mg/L
- Converting this to moles of O₂ gives 0.1366 moles O₂ (= 4.37/32)
- The change in ammonium (or nitrate) concentration is 0.955 mg/L
- Converting this to moles of N gives 0.0682 moles of N (= 0.955/14)

The number of moles of dissolved oxygen consumed (0.137) is twice that the number of moles of N transformed from ammonium to nitrate (0.0682), to two decimal places. This is consistent with Equation E.2.

A full WQ Module mass balance is presented in Appendix Q.

E.3 Denitrification

Denitrification is the pelagic biological reduction of nitrate to free nitrogen gas, N₂. This typically occurs as a result of microbial oxygen stripping from nitrate in low dissolved oxygen environments. It occurs through a series of intermediate stages, but is typically represented as a single-step process with a governing denitrification rate. This rate is computed within the WQ Module via either Equation E.5 or Equation E.6. These are identical other than their treatment of the influence of dissolved oxygen on denitrification, which is either Michaelis-Menten or exponential, respectively. Unlike nitrification, denitrification includes the influence of nitrate concentration in both rate calculations, again in a Michaelis-Menten form.

$$R_{denit\langle computed \rangle}^{NO_3} = R_{denit}^{NO_3} \times \frac{K_{denit-O_2-MM}^{NO_3}}{K_{denit-O_2-MM}^{NO_3} + [DO]} \times [\theta_{denit}^{NO_3}]^{(T-20)} \times \frac{[NO_3]}{K_{denit-NO_3}^{NO_3} + [NO_3]} \quad (E.5)$$

$$R_{denit\langle computed \rangle}^{NO_3} = R_{denit}^{NO_3} \times \underbrace{e^{\left[\frac{-[DO]}{K_{denit-O_2-exp}^{NO_3}} \right]}}_{\text{Influence of oxygen}} \times \underbrace{[\theta_{denit}^{NO_3}]^{(T-20)}}_{\text{Influence of temperature}} \times \underbrace{\frac{[NO_3]}{K_{denit-NO_3}^{NO_3} + [NO_3]}}_{\text{Influence of nitrate}} \quad (E.6)$$

$R_{denit}^{NO_3}$ is the user specified nitrate denitrification rate at 20°C and without the influence of dissolved oxygen, and $[DO]$ and $[NO_3]$ are the ambient dissolved oxygen and nitrate concentrations respectively. If the Michaelis-Menten oxygen model is used then $K_{denit-O_2-MM}^{NO_3}$ is the half saturation concentration of oxygen for denitrification. If the exponential model is used then $K_{denit-O_2-exp}^{NO_3}$ is the dissolved oxygen concentration that normalises (i.e. non-dimensionalises) the ambient oxygen concentration used in Equation E.6. Equation E.5 is the default. Finally, $\theta_{denit}^{NO_3}$ is the temperature coefficient for denitrification of nitrate, T is ambient water temperature, and $K_{denit-NO_3}^{NO_3}$ is the Michaelis-Menten half saturation nitrate concentration that influences denitrification in both Equation E.5 and Equation E.6. $K_{denit-NO_3}^{NO_3}$ is the nitrate concentration for which the computed denitrification rate is half the user specified rate, at 20°C and with no influence of ambient dissolved oxygen concentration. It is not user definable, but hardwired to a value of 0.07 mg/L of nitrate (5.0 mmol/m³).

The computed denitrification rate from Equation E.5 or Equation E.6 is then multiplied by ambient nitrate concentration to compute the flux of nitrate to free nitrogen gas at each model timestep in each model cell via Equation E.7.

$$F_{denit\langle computed \rangle}^{NO_3} = R_{denit\langle computed \rangle}^{NO_3} \times [NO_3] \quad (E.7)$$

Unlike nitrification, denitrification does not produce or consume dissolved oxygen. It does, however, consume nitrate and therefore presents a feedback loop in Equation E.5 through Equation E.7.

The demonstration model was executed over two suites of identical simulations that varied temperature from one simulation to the next, with the first suite using Equation E.5 and the second suite using Equation E.6. Only denitrification

was turned on, and constant values for $R_{denit}^{NO_3}$ (1.5/day - a deliberately very large value was chosen to demonstrate trends), $K_{denit-O_2}^{NO_3}$ (4 mg/L) and $K_{denit-NO_3}^{NO_3}$ (15.5 mg/L) were set. Temperature coefficients were set to 1.05. The predicted temporal evolution of water column nitrate concentrations in these simulation pairs are provided in Figure E.4.

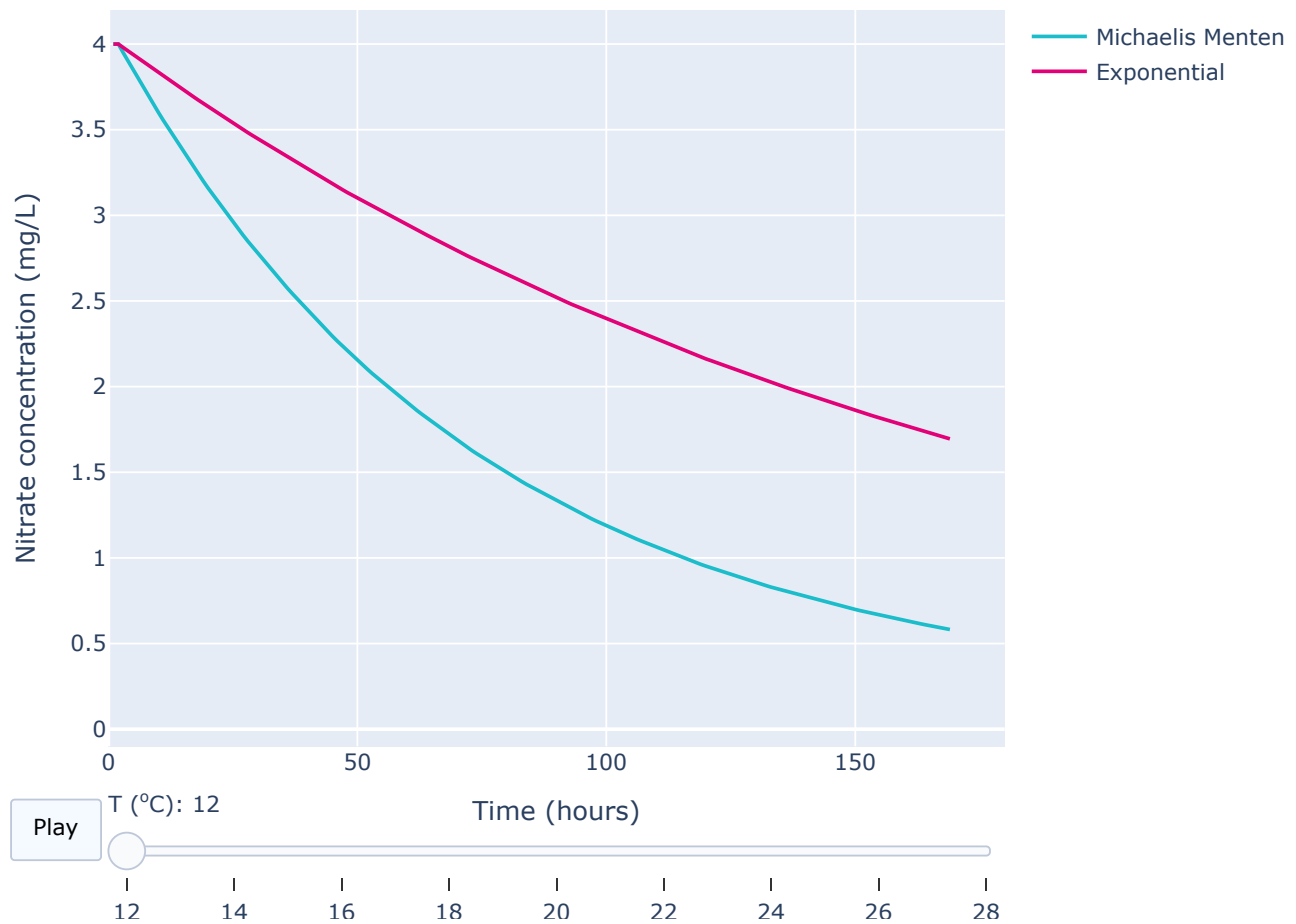


Figure E.4: Move the slider to see the effect of changing temperature on the concentrations of nitrate, where two different denitrification models are used

The figure demonstrates the expected behaviour, where nitrate is consumed in a non-linear manner. The different models produce different drawdown rates, also as expected. In this example, these differences are substantial.

The same two suites of demonstration models were also used to illustrate the influence of varying $K_{denit-O_2}^{NO_3}$ (instead of temperature) on denitrification. All set ups from the models used above were retained, other than setting ambient water temperature to constant at 20 °C, and allowing $K_{denit-O_2}^{NO_3}$ to vary. The predicted temporal evolution of water column nitrate concentrations in these demonstration model simulation pairs are provided in Figure E.5.

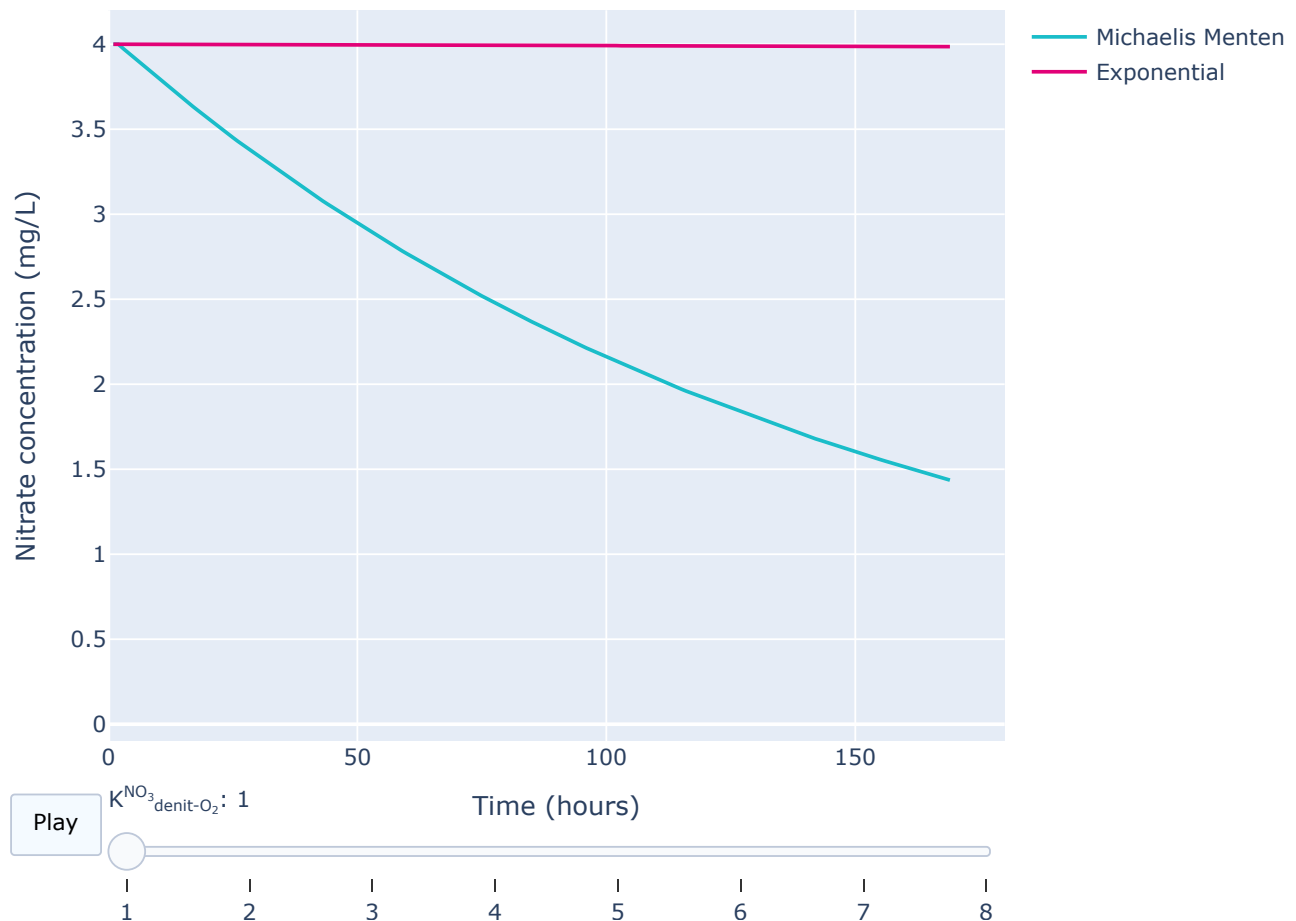
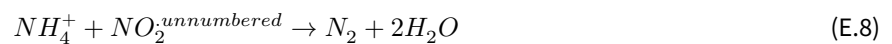


Figure E.5: Move the slider to see the effect of changing $K_{denit-O_2}^{NO_3}$ on the concentrations of nitrate, where two different denitrification models are used

Substantial differences in the prediction of nitrate concentrations is again observed, especially at lower half saturation concentrations.

E.4 Anaerobic oxidation of ammonium

Anaerobic oxidation of ammonium (also referred to as anammox) is the microbial conversion of ammonium and nitrite to free nitrogen gas in low dissolved oxygen environments. Oxygen for this process is stripped from nitrite. The equation representing this process is as follows.



NH_4^+ and $NO_2^{unnumbered}$ are ammonium and nitrite, respectively, and N_2 is free nitrogen gas. In the absence of simulating nitrite, the WQ Module assumes that nitrite and nitrate are related (only at dissolved oxygen concentrations below 0.1 mg/L) as follows.

$$[NO_2] = [NO_3] \times \left(1.0 - \frac{[DO]}{0.1 + [DO]} \right) \quad (E.9)$$

$[NO_2]$, $[NO_3]$ and $[DO]$ are the ambient nitrite, ammonium and dissolved oxygen concentrations, respectively. The anammox flux to free nitrogen gas N at each model timestep in each model cell that has an ambient dissolved oxygen concentration less than 0.1 mg/L is computed as per Equation E.10.

$$F_{anmx}^{N_2}(\text{computed}) = k_{anmx}^{N_2} \times \frac{[NH_4]}{K_{anmx-NH_4}^{N_2} + [NH_4]} \times \frac{[NO_2]}{K_{anmx-NO_2}^{N_2} + [NO_2]} \quad (\text{E.10})$$

$k_{anmx}^{N_2}$ is the user specified anaerobic volumetric mass oxidation rate without the influence of ammonium or nitrite, $K_{anmx-NH_4}^{N_2}$ and $K_{anmx-NO_2}^{N_2}$ are the Michaelis-Menten half saturation ammonium and nitrite concentrations for anammox respectively, and $[NH_4]$ and $[NO_2]$ are the ambient ammonium and nitrite concentrations, respectively. For ambient conditions that have dissolved oxygen concentrations greater than 0.1 mg/L, the anammox rate is set to zero.

E.5 Dissimilatory reduction of nitrate to ammonium

Dissimilatory reduction of nitrate to ammonium (also referred to as DRNA) is the microbial conversion of nitrate to ammonium. Dissolved oxygen is not consumed in this process. The WQ Module assumes the number of moles of nitrate-N consumed is the same as the number of ammonium-N moles produced. The DRNA rate is computed within the WQ Module via Equation E.11.

$$R_{DRNA}^{NO_3}(\text{computed}) = R_{DRNA}^{NO_3} \times \frac{K_{DRNA-O_2}^{NO_3}}{K_{DRNA-O_2}^{NO_3} + [DO]} \quad (\text{E.11})$$

$R_{DRNA}^{NO_3}$ is the user specified rate of dissimilatory reduction of nitrate to ammonium without the influence of oxygen, $K_{DRNA-O_2}^{NO_3}$ is the Michaelis-Menten half saturation dissolved oxygen concentration for DRNA, and $[DO]$ is the ambient dissolved oxygen concentration.

The computed DRNA rate from Equation E.11 is multiplied by ambient nitrate concentration to compute the flux to ammonium at each model timestep in each model cell as per Equation E.12.

$$F_{DRNA}^{NO_3}(\text{computed}) = R_{DRNA}^{NO_3}(\text{computed}) \times [NO_3] \quad (\text{E.12})$$

Although not recommended, the influence of oxygen in all the processes described in Section E.1 to Section E.5 can be removed by setting the command `oxygen == off` in the nitrogen model block. This switch applies to sediment flux, nitrification and denitrification. Anammox and DRNA will be switched off entirely if this command is issued.

E.6 Wet deposition of inorganic nitrogen

Wet deposition of inorganic nitrogen includes the pluvial delivery of both ammonium and nitrate to the water column. A global total inorganic nitrogen concentration in rainfall is specifiable, together with the proportion of that total that is nitrate. From this, the WQ Module computes ammonium and nitrate concentrations (Equation E.13 and Equation E.14, respectively).

$$[NH_4]_{rain} = [TN]_{rain} \times (1 - f_{TN}^{NO_3}) \quad (\text{E.13})$$

$$[NO_3]_{rain} = [TN]_{rain} \times f_{TN}^{NO_3} \quad (\text{E.14})$$

$[TN]_{rain}$ and $f_{TN}^{NO_3}$ are the concentration of total nitrogen in rain and the fraction of that total that is nitrate, respectively. The WQ Module separately multiplies $[NH_4]_{rain}$ and $[NO_3]_{rain}$ by each timestep's rainfall depth and corresponding model surface area(s) to compute the wet mass flux of ammonium and nitrate (Equation E.15 and Equation E.16, respectively). These masses are added to the uppermost model layer cells and corresponding changes to ambient concentrations computed.

$$F_{atm-wet}^{NH_4} = [NH_4]_{rain} \times \text{Timestep rainfall depth} \times \text{Model area(s)} \quad (\text{E.15})$$

$$F_{atm-wet}^{NO_3} = [NO_3]_{rain} \times \text{Timestep rainfall depth} \times \text{Model area(s)} \quad (E.16)$$

If rainfall depth is specified as being spatially variable (i.e. by application of multiple atmospheric boundary conditions within TUFLOW FV), then $F_{atm-wet}^{NH_4}$ and $F_{atm-wet}^{NO_3}$ will correspondingly vary spatially.

E.7 Dry deposition of inorganic nitrogen

Dry deposition of nitrogen includes the delivery of both ammonium and nitrate to the water column from atmospheric fallout. This fallout is typically thought of as being associated with dust, with the dry fallout dissolving on entry to the water column to become dissolved inorganic nitrogen. A single constant daily deposition rate of total nitrogen is specifiable, and the WQ Module splits this into separate ammonia and nitrate rates using the same fraction applied to the wet deposition total inorganic nitrogen concentration (Section E.6).

$$R_{atm-dry}^{NH_4} = R_{atm-dry}^{TN} \times (1 - f_{TN}^{NO_3}) \quad (E.17)$$

$$R_{atm-dry}^{NO_3} = R_{atm-dry}^{TN} \times f_{TN}^{NO_3} \quad (E.18)$$

$R_{atm-dry}^{TN}$ and $f_{TN}^{NO_3}$ are the user specified rate of dry total inorganic nitrogen deposition, and the fraction that is nitrate, respectively. These individual rates $R_{atm-dry}^{NH_4}$ and $R_{atm-dry}^{NO_3}$ are multiplied by model timestep and the global model surface area to compute the dry mass flux of ammonium and nitrate (Equation E.19 and Equation E.20, respectively). These masses are added to the uppermost model layer cells and corresponding changes to ambient concentrations computed.

$$F_{atm-dry}^{NH_4} = R_{atm-dry}^{NH_4} \times \text{Timestep} \times \text{Global model area} \quad (E.19)$$

$$F_{atm-dry}^{NO_3} = R_{atm-dry}^{NO_3} \times \text{Timestep} \times \text{Global model area} \quad (E.20)$$

This constant dry mass flux for each of ammonium and nitrate is applied globally.

The total atmospheric depositional flux of dissolved inorganic nitrogen (noting that dry atmospheric flux is assumed to dissolve on entry to the water column) is as per Equation E.21.

$$F_{atm-din}^{N}(\text{computed}) = F_{atm-wet}^{NH_4} + F_{atm-wet}^{NO_3} + F_{atm-dry}^{NH_4} + F_{atm-dry}^{NO_3} \quad (E.21)$$

F Processes: inorganic phosphorus

F.1 Sediment FRP flux

Filterable reactive phosphorus (FRP) is exchanged between the water column and sediments via specification of sediment fluxes. This flux is most commonly out of the sediments, i.e. a positive specification of sediment flux. Although it is rare that sediments act as sinks of FRP, WQ Module can be parameterised to allow for this if required.

The user specified rate of FRP flux (which can be spatially varying) is modified by overlying ambient dissolved oxygen concentration (together with a user specified half saturation oxygen concentration) and water temperature. These modifications are simulated via Michaelis-Menten and Arrhenius models, respectively, as per Equation F.1.

$$F_{sed}^{FRP(computed)} = F_{sed}^{FRP} \times \underbrace{\frac{K_{sed-O_2}^{FRP}}{K_{sed-O_2}^{FRP} + [DO]}}_{\text{Influence of oxygen}} \times \underbrace{[\theta_{sed}^{FRP}]^{(T-20)}}_{\text{Influence of temperature}} \quad (F.1)$$

F_{sed}^{FRP} is the user specified FRP sediment flux at 20°C without the influence of dissolved oxygen, $[DO]$ is the overlying dissolved oxygen concentration, $K_{sed-O_2}^{FRP}$ is the user specified half saturation concentration of dissolved oxygen for FRP sediment flux, θ_{sed}^{FRP} is the corresponding temperature coefficient, and T is ambient water temperature.

As per silicate sediment fluxes (see Section D.1), the above equation leads to linearly varying ambient FRP concentrations in the demonstration model when dissolved oxygen concentration, half saturation oxygen concentration and temperature are set to be constant.

A more realistic environmental setting has sediment FRP flux occurring against a background of oxygen concentration drawdown. The demonstration model has been used to illustrate this via execution of a suite of simulations that experience dissolved oxygen drawdown, with $K_{sed-O_2}^{O_2} = 4$ mg/L and each simulation using a different $K_{sed-O_2}^{FRP}$. The FRP sediment flux rate was specified as 400 mg/m²/d and temperature effects were turned off. The predicted temporal evolution of water column FRP concentrations is provided in Figure F.1. Use the “play” button or drag the slider to see how different half saturation concentrations change ambient concentrations.

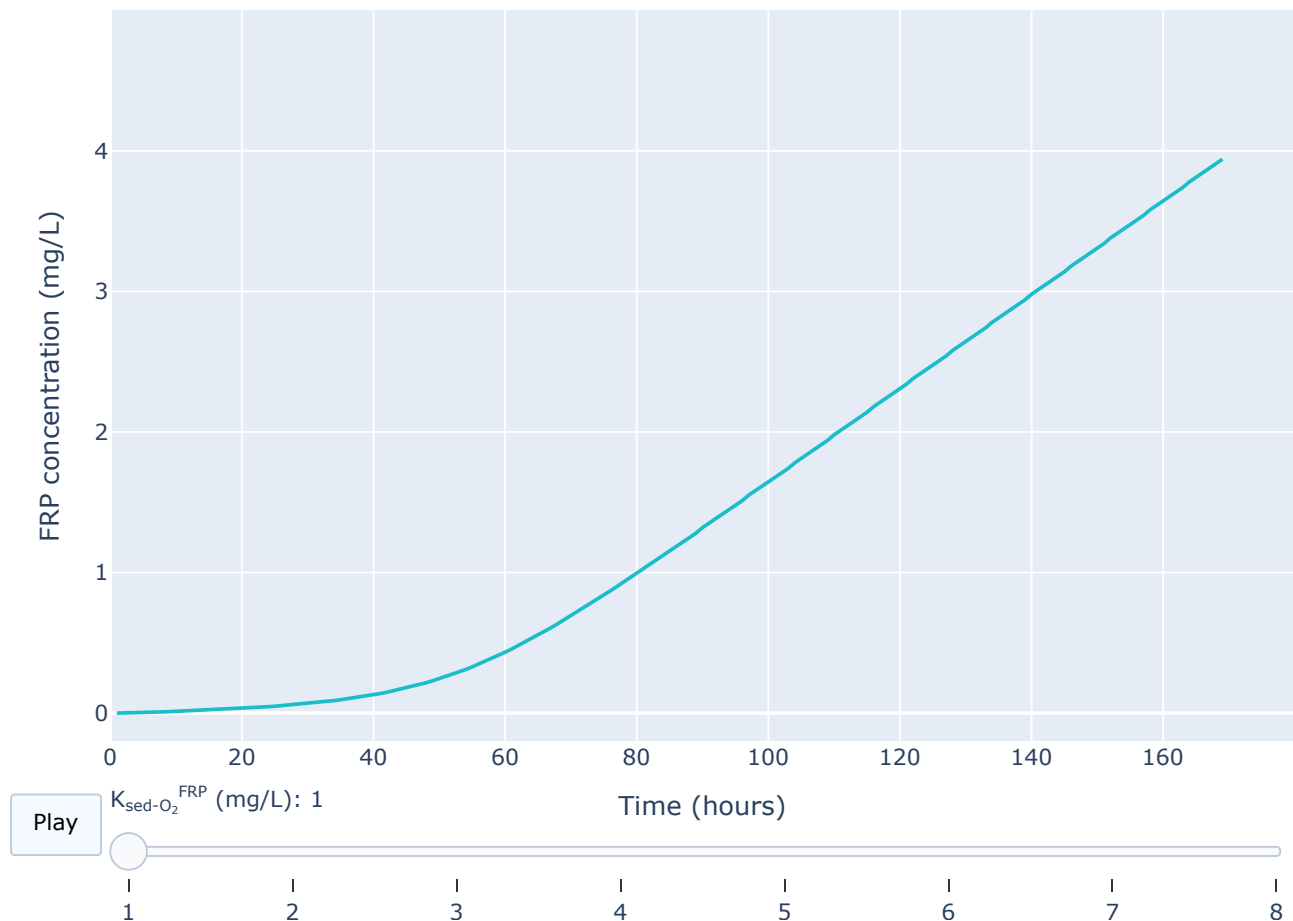


Figure F.1: Move the slider to see the effect of changing the $K_{sed-O_2}^{FRP}$ values on ambient FRP concentrations. Ambient dissolved oxygen is drawn down in time

The rate of FRP flux is also related to ambient water temperature, via the Arrhenius model in Equation F.1. To demonstrate this, the same model above (with time varying dissolved oxygen concentration) was executed at a range of ambient temperatures, but constant half saturation concentrations for oxygen set to 4 mg/L. All temperature coefficients were set to 1.05. The results are provided in Figure F.2. Use the “play” button or drag the slider to see how different ambient temperatures change ambient concentrations.

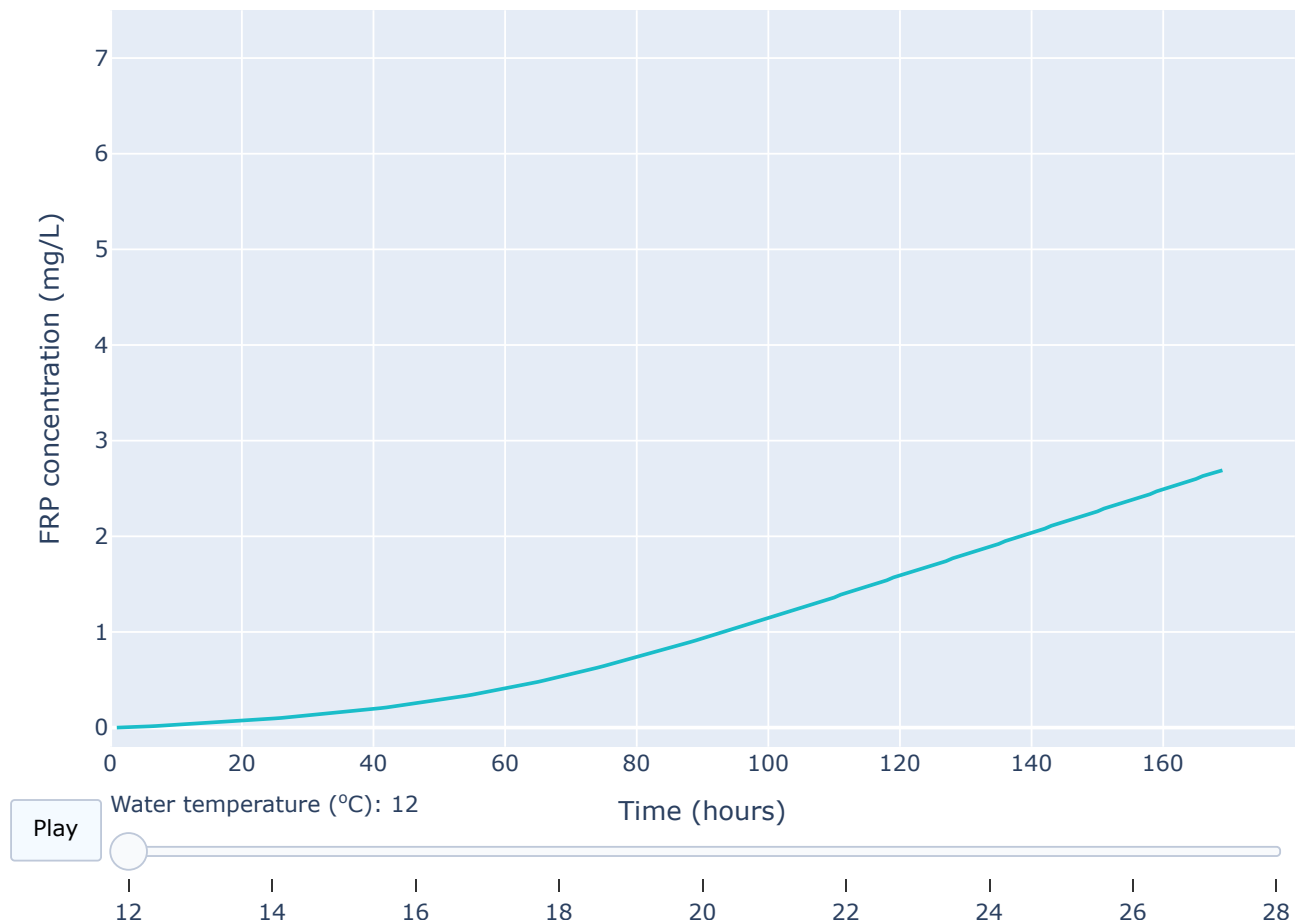


Figure F.2: Move the slider to see the effect of changing the ambient water temperature on the rate of FRP fluxes to water immediately above the sediments, with ambient dissolved oxygen drawdown

The figure shows that as ambient water temperature increases, the rate of increase of FRP concentrations follow suit. This is expected behaviour.

F.2 Wet deposition of inorganic phosphorus

Wet deposition of inorganic phosphorus includes the pluvial delivery of filterable reactive phosphorus to the water column. A global FRP concentration in rainfall is specifiable. The WQ Module multiplies this concentration by each timestep's rainfall depth and corresponding model surface area(s) to compute the wet mass flux of FRP over each timestep (Equation F.2).

$$F_{atm-wet}^{FRP} = [FRP]_{rain} \times \text{Timestep rainfall depth} \times \text{Model area} \quad (F.2)$$

$[FRP]_{rain}$ is the specified rainfall concentration of FRP. This mass is added to the uppermost model layer cells and corresponding changes to ambient FRP concentrations computed.

If rainfall depth is specified as being spatially variable (i.e. by application of multiple atmospheric boundary conditions within TUFLOW FV), then $F_{atm-wet}^{FRP}$ will correspondingly vary spatially.

F.3 Dry deposition of inorganic phosphorus

Dry deposition of inorganic phosphorus includes the delivery of adsorbed FRP to the water column from atmospheric dust fallout. A constant daily mass loading rate of adsorbed FRP is specifiable, and the WQ Module multiplies this rate by model timestep and the global model surface area to compute the mass flux of adsorbed FRP (Equation F.3). This

mass is added to the uppermost model layer cells and corresponding changes to ambient concentrations computed. Dry deposition is only included in calculations if adsorbed FRP is simulated.

$$F_{atm-dry}^{FRPads} = R_{atm-dry}^{FRPads} \times \text{Timestep} \times \text{Global model area} \quad (\text{F.3})$$

$R_{atm-dry}^{FRPads}$ is the user specified rate of adsorbed FRP atmospheric fallout. One (constant) mass flux is applied globally. This dry deposition is only applied if FRP adsorption is simulated, and if this is the case, then this introduction of dry deposited FRP is assigned to the adsorbed FRP computed variable. If adsorbed FRP is not included in a simulation, then dry deposition of FRP will be ignored.

The total atmospheric depositional flux of inorganic phosphorus is as per Equation F.4.

$$F_{atm-dip}^{P(\text{computed})} = F_{atm-wet}^{FRP} + F_{atm-dry}^{FRPads} \quad (\text{F.4})$$

F.4 Adsorption and desorption

At each timestep and within each active computational cell, the WQ Module distributes the total FRP mass between dissolved FRP and adsorbed FRP if the phosphorus adsorption constituent model is used. Total FRP is conserved via Equation F.5.

$$[FRP]_{tot} = [FRPads] + [FRP] \quad (\text{F.5})$$

$[FRP]_{tot}$ is the total FRP available for distribution between dissolved and adsorbed states, and $[FRPads]$ and $[FRP]$ are the ambient adsorbed and dissolved FRP concentrations, respectively.

The distribution between adsorbed and dissolved FRP concentrations is computed within the WQ Module via either a linear or quadratic model. These offer alternative approaches to simulating the distribution of total FRP between adsorbed and free states.

F.4.1 Linear model

Equation F.6 is the linear adsorption model, and the default.

$$\left. \begin{aligned} [FRPads] &= \left(\frac{K_{ads-L}^{FRP} \times [SS]}{1 + K_{ads-L}^{FRP} \times [SS]} \right) \times [FRP]_{tot} \\ [FRP] &= \left(\frac{1}{1 + K_{ads-L}^{FRP} \times [SS]} \right) \times [FRP]_{tot} \end{aligned} \right\} \quad (\text{F.6})$$

$[SS]$ is the sum of suspended sediment concentrations of sediment fractions that have been designated as able to adsorb FRP and K_{ads-L}^{FRP} is the linear sorption partitioning coefficient.

Figure F.3 provides an indicative representation of the general form of the linear relationship, for assumed total FRP (0.1 mg/L) and SS (5mg/L) concentrations.

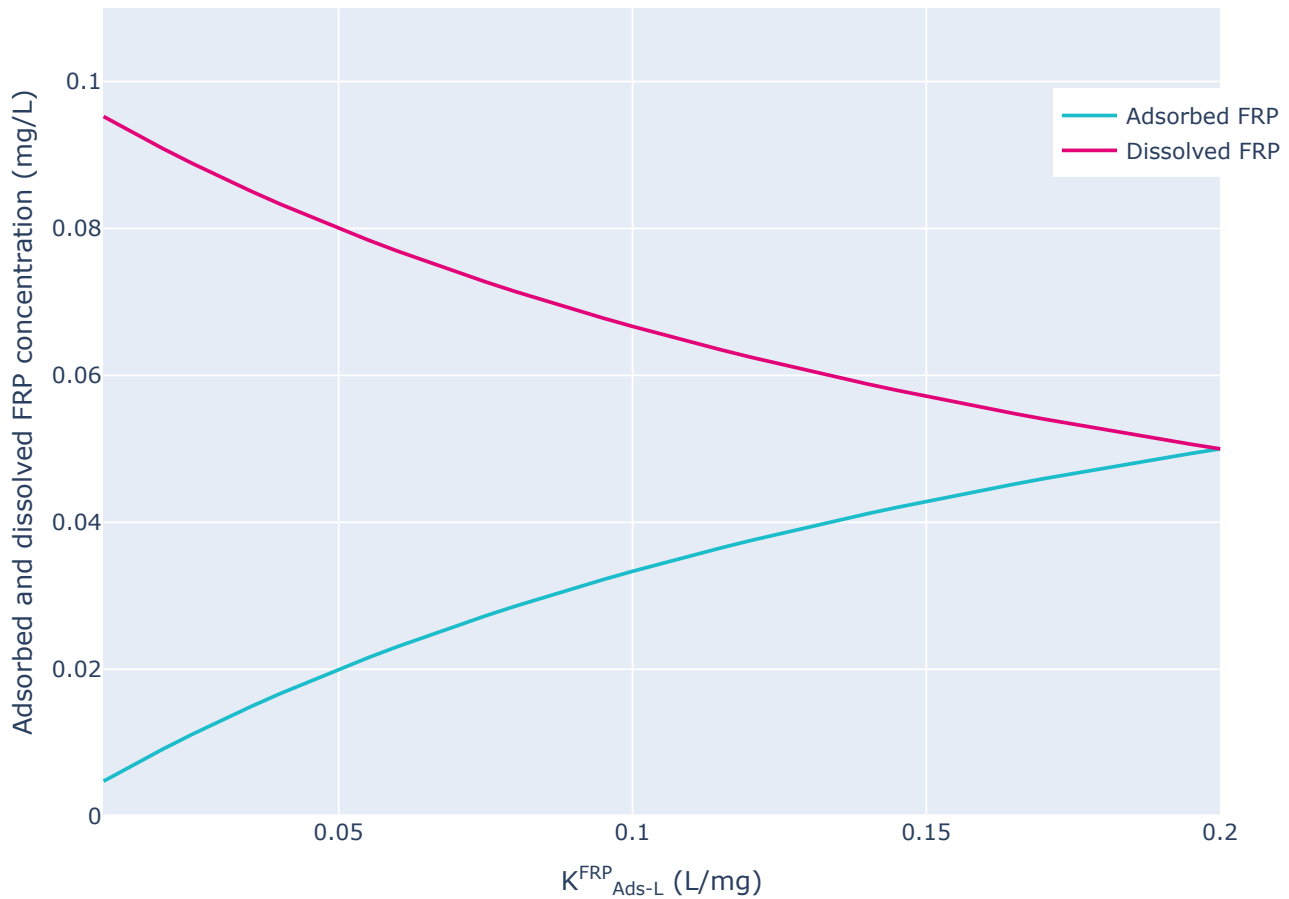


Figure F.3: The change in distribution of dissolved and adsorbed FRP under the linear adsorption model. This figure has no slider bar

As a guide, Equation F.6 has that if $K_{ads-L}^{FRP} \times [SS]$ has a value of 1, then an equal (50:50) proportioning of free and adsorbed FRP will result. This guide can be useful if ambient suspended sediment concentrations are known - even approximately - in advance.

F.4.2 Quadratic model

Equation F.7 is the quadratic adsorption model.

$$\left. \begin{aligned}
 [FRP_{ads}] &= \frac{1}{2} \times \left[\left([FRP]_{Tot} + \frac{1}{K_{ads-Q}^{FRP}} + ([SS] \times Q_{max}^{FRP}) \right) - C \right] \\
 [FRP] &= \frac{1}{2} \times \left[\left([FRP]_{Tot} - \frac{1}{K_{ads-Q}^{FRP}} - ([SS] \times Q_{max}^{FRP}) \right) + C \right]
 \end{aligned} \right\} \quad (F.7)$$

$$C = \sqrt{\left([FRP]_{Tot} + \frac{1}{K_{ads-Q}^{FRP}} - ([SS] \times Q_{max}^{FRP}) \right)^2 + \left(\frac{4.0 \times [SS] \times Q_{max}^{FRP}}{K_{ads-Q}^{FRP}} \right)}$$

$[SS]$ is again the sum of suspended sediment concentrations of sediment fractions that have been designated as able to adsorb FRP, K_{ads-Q}^{FRP} is the ratio of adsorption and desorption rate coefficients and Q_{max}^{FRP} is the maximum adsorption capacity of suspended sediment, for FRP.

Figure F.4 provides an indicative representation of the general form of the quadratic relationship, again for assumed total FRP (0.1 mg/L) and SS (5mg/L) concentrations.

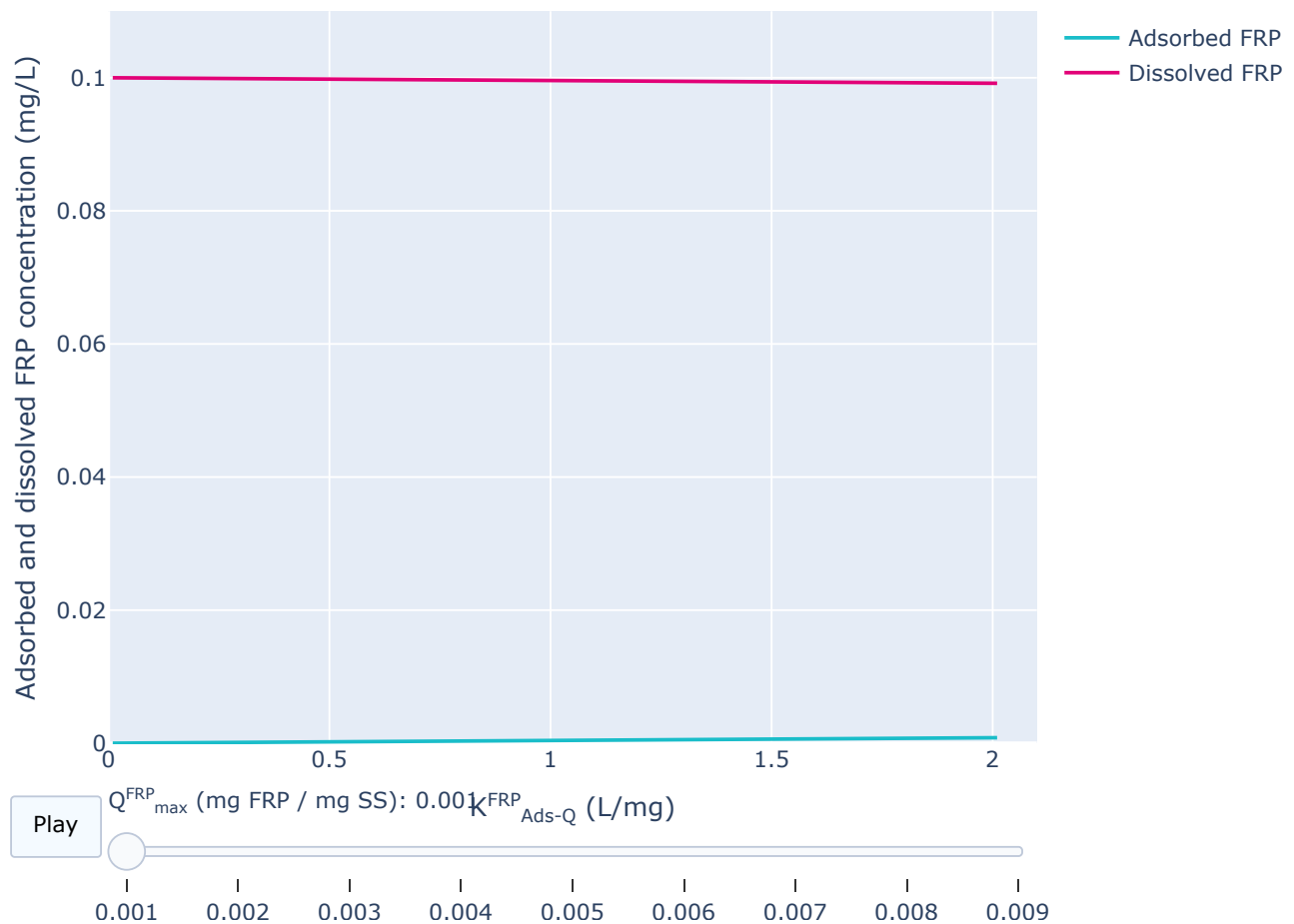


Figure F.4: The change in distribution of dissolved and adsorbed FRP under the quadratic adsorption model

The parameters used to prepare the above figures were deliberately chosen to illustrate the different behaviour that can result from these two models. This underscores the need to make careful decisions regarding the selection of an adsorption model.

F.5 Settling

At each timestep and within each active computational cell, the WQ Module computes the mass of adsorbed FRP that has settled either through the water column or onto the bed, using the settling velocity provided by the user. The limitations of this approach are recognised and future releases of the WQ Module will link this process directly to the settling and resuspension calculations of the TUFLOW FV ST Module.



G Processes: phyto general

G.1 General

Any number of phytoplankton groups may be simulated within the WQ Module, however the majority of environmental modelling applications rarely require (or have data to justify) including more than a relatively small number. Each phytoplankton group can have its properties set independently, where these properties typically relate to interaction with temperature, light, salinity and nutrients.

The WQ Module offers two constituent models for the simulation of phytoplankton. These are referred to as basic and advanced, and are primarily differentiated on the basis of whether internal nutrients are simulated, as:

- Constituent model basic does not include simulation of internal phytoplanktonic nutrients
- Constituent model advanced does include simulation of internal phytoplanktonic nutrients

This constituent model naming is intended to reflect a view that excluding simulation of internal nutrients is a simpler, more rudimentary, approach to phytoplankton modelling. Similarly, internal nutrient simulation generally requires specification of a larger suite of parameters than when the process is excluded, so is often considered to be a more complex and involved approach to phytoplankton simulation.

A WQ Module simulation can include any combination of these two constituent models if multiple phytoplankton groups are simulated. For example, if three phytoplankton groups are to be simulated, two groups could be set to use the basic constituent model, and one to use the advanced constituent model.

Where WQ Module calculations are completed differently between these two constituent models, their respective approaches are presented in a complementary but distinct manner following.

G.2 Units

Phytoplankton is accounted within the WQ Module in units of carbon, however carbon need not be explicitly simulated within the WQ Module as either inorganic (not yet available) or organic (labile and/or refractory) to support this approach. If this is the case, then uptake or loss of carbon by phytoplankton is still computed as it is the basis for accounting and reporting phytoplankton concentrations. The associated carbon sources and sinks that interact with phytoplankton carbon however, are assumed to be large and are not specifically accounted for as computed variables. A user specified (or default) conversion ratio between mg of carbon and mg of chlorophyll *a*, X_{cc}^{phy} , is used to present carbon model outputs in units of $\mu\text{g/L}$ chlorophyll *a* when necessary.



H Processes: phyto biomass rates

The rates that determine the temporal evolution of a phytoplankton group's biomass are primary productivity, respiration, exudation and settling. In general terms these processes can be thought of as follows:

- Primary productivity is the consumption of carbon and the generation of oxygen and carbohydrate due to photosynthesis. Photosynthetically active radiation catalyses this process so it occurs only during daylight hours. This process is also referred to as growth or gross primary productivity
- Respiration is the consumption of oxygen and stored carbohydrate and the production of carbon. This can be thought of as the reverse of primary productivity. Respiration dominates phytoplankton dynamics during nighttime hours, although it generally still operates during the daytime
- Exudation (also referred to as photo exudation) is the loss of phytoplankton biomass as a result of primary productivity
- Settling is the physical settling of phytoplankton, including motility

The general form of the phytoplankton flux relationship for any given computational cell is therefore given by Equation H.1.

$$F^{phy} = \text{Primary productivity} - f(\text{Respiration, Exudation}) - \text{Settling} \quad (\text{H.1})$$

f represents functions described in Appendix K. The fundamental rates in Equation H.1 - primary productivity, respiration, exudation and settling - are described following.

H.1 Primary productivity

The primary productivity rate is computed in a series of stages within the WQ Module, where the combination of these stages used for any given phytoplankton group depends on group configuration. These stages are described below. For clarity, supporting functions nested within primary productivity rate calculations (such as limitation functions) are initially presented in passing, but are cross referenced to detailed descriptions in subsequent Appendices.

The rate of primary productivity (often referred to as just productivity or growth rate) of a phytoplankton group is a /day rate. It is computed initially within the WQ Module as per Equation H.2.

$$R_{prod(computed)}^{phy} = R_{prod}^{phy} \times L_T^{phy} \times \min(L_{lght}^{phy}, L_{nit}^{phy}, L_{phs}^{phy}, L_{sil}^{phy}) \quad (\text{H.2})$$

For each phytoplankton group, R_{prod}^{phy} is the user specified (or default) phytoplankton productivity (growth) rate at 20°C with no light, temperature, salinity, silicate or nutrient limitation, and L_T^{phy} , L_{lght}^{phy} , L_{nit}^{phy} , L_{phs}^{phy} , L_{sil}^{phy} are the computed limitation functions for water temperature, light, nitrogen, phosphorus and silicate, respectively. These functions, when appropriate, act to modify R_{prod}^{phy} , noting that only L_T^{phy} always does so. The other limitation functions in Equation H.2 act collectively, with only the most limiting (i.e. the smallest function value) of L_{lght}^{phy} , L_{nit}^{phy} , L_{phs}^{phy} and L_{sil}^{phy} being selected to also multiplicatively modify R_{prod}^{phy} with L_T^{phy} .

If nitrogen fixing is implemented, then the productivity rate computed in Equation H.2 is further modified as per Equation H.3.

$$R_{prod(computed)}^{phy} = R_{prod(computed)}^{phy} \times (f_{nfix}^{phy} + L_{nit}^{phy} \times (1.0 - f_{nfix}^{phy})) \quad (\text{H.3})$$

f_{nfix}^{phy} accounts for the metabolic cost of nitrogen fixing on primary productivity and is the user specified (or default) reductive factor applied to productivity under full nitrogen fixing conditions. Specifically:

- Full nitrogen fixing occurs when L_{nit}^{phy} is zero (i.e. no water column nitrogen is available for uptake), and Equation H.3 then has $R_{prod(computed)}^{phy}$ reduced by the factor f_{nfix}^{phy}

- No nitrogen fixing occurs when L_{nit}^{phy} is one (i.e. excess water column nitrogen is available for uptake), and Equation H.3 then has $R_{prod(computed)}^{phy}$ unchanged

Salinity limitation of primary productivity is not mandatory, and can be switched on and off by the user, or equally set to be an enhancer of respiration rather than reducer of productivity. If salinity limitation of productivity is implemented, then the $R_{prod(computed)}^{phy}$ computed above is further modified as per Equation H.4.

$$R_{prod(computed)}^{phy} = R_{prod(computed)}^{phy} \times L_{sal-pp}^{phy} \quad (H.4)$$

L_{sal-pp}^{phy} is the limitation on primary productivity due to salinity and is between zero and one, as per the other limitation functions noted above.

Once the rate of primary productivity has been computed by applying Equation H.2, and potentially Equation H.3 and Equation H.4, the corresponding flux of carbon (i.e. phytoplankton growth) to a phytoplankton group is computed as per Equation H.5.

$$F_{prod(computed)}^{phy} = R_{prod(computed)}^{phy} \times [PHY] \quad (H.5)$$

$[PHY]$ is the ambient phytoplankton group concentration. These fluxes are summed over all simulated phytoplankton groups to compute the community primary productivity, $F_{prod(computed)}^{comm}$.

The corresponding fluxes of nitrogen due to this primary productivity are described by Equation J.2 (basic model) and Equation J.4 (advanced model). Similarly, the corresponding fluxes of phosphorus are described by Equation J.7 (basic model) and Equation J.8 (advanced model). The same diagnostic variable name is used to report these fluxes, regardless of the phytoplankton model used.

The WQ Module uses a minimum concentration $[PHY]_{min}$ to maintain phytoplankton concentrations above zero. This is because if concentrations decrease to zero, then by Equation H.5, phytoplankton fluxes (and therefore concentrations) will remain at zero regardless of computed primary productivity rates.

H.2 Respiration

The respiration rate is computed in a series of stages within the WQ Module, where the combination of these stages used for any given phytoplankton group depends on group configuration. These stages are described below. For clarity, supporting functions nested within respiration rate calculations (such as limitation functions) are initially presented in passing, but are cross referenced to detailed descriptions in subsequent sections.

The rate of respiration of a phytoplankton group is a /day rate. It is computed initially within the WQ Module as per Equation H.6.

$$R_{resp(computed)}^{phy} = R_{resp}^{phy} \times \underbrace{\left[\theta_{resp}^{phy} \right]^{(T-20)}}_{\text{Influence of temperature}} \quad (H.6)$$

R_{resp}^{phy} is the user specified phytoplankton respiration rate at 20°C, θ_{resp}^{phy} is the temperature coefficient for respiration, and T is ambient water temperature. Figure H.1 presents the influence of θ_{resp}^{phy} on R_{resp}^{phy} , as a function of temperature.

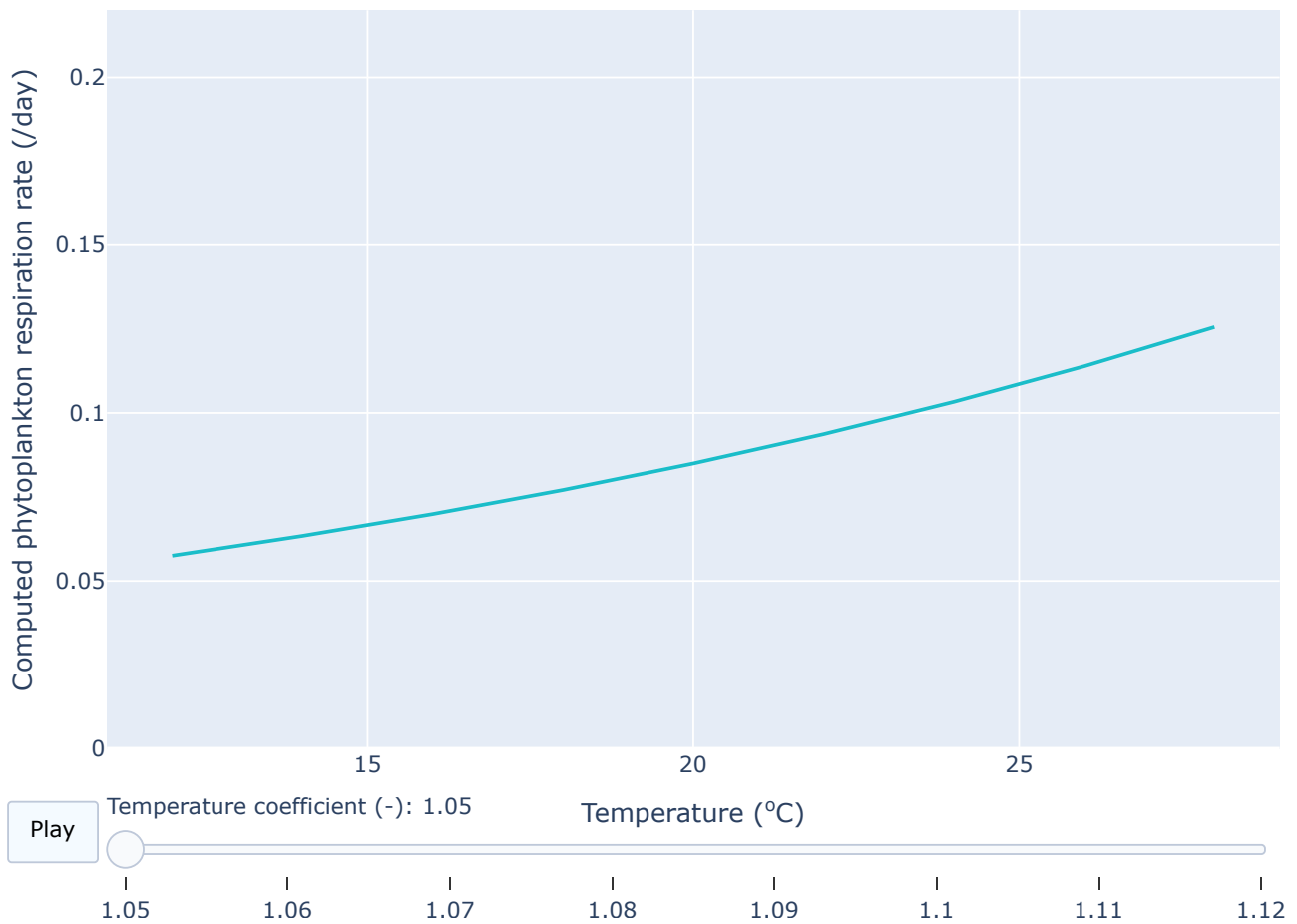


Figure H.1: Move the slider to see the effect of changing temperature coefficient on the computed phytoplankton respiration rate

As for primary productivity, salinity limitation of respiration is not mandatory, and can be switched on and off by the user. If salinity limitation of respiration is implemented, then the $R_{resp(computed)}^{phy}$ computed above is further modified as per Equation H.7.

$$R_{resp(computed)}^{phy} = R_{resp(computed)}^{phy} \times L_{sal-r}^{phy} \quad (H.7)$$

L_{sal-r}^{phy} is the limitation function on respiration due to salinity, and is always greater than one. This limitation function can therefore be conceptualised as a respiration enhancer: it acts to reduce biomass via increasing respiration rather than reducing primary productivity. Salinity limitation is applied to only one of primary production (Section H.1) or respiration, depending on the salinity limitation model selected, and not both.

If a group's ambient phytoplankton concentration is less than the user defined (or default) minimum concentration $[PHY]_{min}$, then the respiration rate is set to zero.

Once the respiration rate has been computed, the corresponding flux of carbon (i.e. phytoplankton respiration) from a phytoplankton group due only to respiration (i.e. excluding mortality and excretive losses) is as per Equation H.8.

$$F_{resp(computed)}^{phy} = R_{resp(computed)}^{phy} \times f_{true-resp}^{phy} \times [PHY] \quad (H.8)$$

$f_{true-resp}^{phy}$ is the user specified (or default) fraction of respiration that corresponds to the generation of energy via consumption of stored chlorophyll *a* (i.e. the fraction that does not result in excretive or mortality losses) and $[PHY]$ is the ambient phytoplankton group concentration. For a given phytoplankton group, net productivity is calculated as primary productivity, less the flux computed in Equation H.8 (i.e. respiration due only to energy generation). These net productivity fluxes are summed over the number of simulated phytoplankton groups (i.e. $n = 1$ to num_phy) to compute the community net primary productivity as per Equation H.9.

$$F_{netprod(computed)}^{comm} = \sum_{n=1}^{num_phy} [F_{prod(computed)}^{phy_n} - F_{resp(computed)}^{phy_n}] \quad (H.9)$$

The respiration fluxes of nitrogen and phosphorus corresponding to Equation H.8 are as per Equation H.10 and Equation H.11, respectively.

$$F_{resp-N(computed)}^{phy} = R_{resp(computed)}^{phy} \times f_{true-resp}^{phy} \times [IN] \quad (H.10)$$

$$F_{resp-P(computed)}^{phy} = R_{resp(computed)}^{phy} \times f_{true-resp}^{phy} \times [IP] \quad (H.11)$$

$[IN]$ and $[IP]$ are the internal phytoplankton nitrogen and phosphorus concentrations, respectively. These are either constant ratios of nitrogen and phosphorus to phytoplankton biomass (i.e. the basic phytoplankton model) or computed variables (i.e. the advanced phytoplankton model), and the WQ Module will use the appropriate value based on the phytoplankton model deployed, on a group by group basis.

H.3 Exudation

The exudation rate of a phytoplankton group is a /day rate. It is computed within the WQ Module as per Equation H.12.

$$R_{exud(computed)}^{phy} = R_{prod(computed)}^{phy} \times f_{exud}^{phy} \quad (H.12)$$

$R_{prod(computed)}^{phy}$ is the previously computed phytoplankton primary production rate (Equation H.2, and potentially Equation H.3 and Equation H.4), and f_{exud}^{phy} is the user defined (or default) fraction of primary production lost to exudation. This exudation loss is a linear function.

If a group's ambient phytoplankton concentration is less than the user defined (or default) minimum concentration $[PHY]_{min}$, then the exudation rate is set to zero.

H.4 Settling

The settling rate V_{settle}^{phy} (also referred to as motility) of a phytoplankton group is applied within the WQ Module for each phytoplankton group, prior to the corresponding primary production, respiration and exudation rate calculations. There are several phytoplankton settling models available within the WQ Module. These are described following, and once the settling rate has been computed, the flux (loss) of phytoplankton carbon to the sediments (i.e. from the bottom cell of each computational water column only) is computed for each phytoplankton group via Equation H.13.

$$F_{sedmtn(computed)}^{phy} = \frac{V_{settle}^{phy}}{dz} \times [PHY] \quad (H.13)$$

dz is the relevant cell thickness, and divides the flux to produce a per volume result for consistency with other corresponding diagnostics (such as mortality). These fluxes are summed over all simulated phytoplankton groups to compute the community sedimentation rate, $F_{sedmtn(computed)}^{comm}$. The latter is in per area units.

The corresponding sedimentation flux of phytoplanktonic nitrogen is computed via either Equation H.14 (basic model) or Equation H.15 (advanced model). The same diagnostic variable name is used to report these fluxes, regardless of the phytoplankton model used.

$$F_{sedmtn-N(computed)}^{phy} = \frac{V_{settle}^{phy}}{dz} \times [PHY] \times X_{N-C-con}^{phy} \quad (H.14)$$

$X_{N-C-con}^{phy}$ is the specified (or default) constant ratio of internal nitrogen to carbon in the phytoplankton group being considered.

$$F_{sedmntn-N}^{phy} = \frac{V_{settle}^{phy}}{dz} \times [IN] \quad (H.15)$$

$[IN]$ is the internal phytoplankton nitrogen concentration.

The corresponding sedimentation flux of phytoplanktonic phosphorus is computed via either Equation H.16 (basic model) or Equation H.17 (advanced model). The same diagnostic variable name is used to report these fluxes, regardless of the phytoplankton model used.

$$F_{sedmntn-P}^{phy} = \frac{V_{settle}^{phy}}{dz} \times [PHY] \times X_{P-C-con}^{phy} \quad (H.16)$$

$X_{P-C-con}^{phy}$ is the specified (or default) constant ratio of internal phosphorus to carbon in the phytoplankton group being considered.

$$F_{sedmntn-P}^{phy} = \frac{V_{settle}^{phy}}{dz} \times [IP] \quad (H.17)$$

$[IP]$ is the internal phytoplankton phosphorus concentration.

H.4.1 None

In this model, phytoplankton settling V_{settle}^{phy} is set to zero and phytoplankton are simply advected by the hydrodynamic flow field.

H.4.2 Constant

In this model, phytoplankton settling V_{settle}^{phy} is set to a constant value, and phytoplankton are settled at this velocity. A negative specification of this quantity corresponds to a downwards settling velocity.

H.4.3 Constant with density correction

In this model, phytoplankton settling V_{settle}^{phy} is set to a constant value, and phytoplankton are settled at this velocity, but corrected for ambient water density effects, as per Equation H.18.

$$V_{sett(computed)}^{phy} = V_{settle}^{phy} \times \frac{\mu_{20} \times \rho_w}{\mu \times \rho_{w20}} \quad (H.18)$$

V_{settle}^{phy} is the specified settling rate (velocity) at 20°C, μ and ρ_w are the ambient water dynamic viscosity (in Ns/m²) and density (in kg/m³), respectively, and μ_{20} and ρ_{w20} are the dynamic viscosity and density of freshwater at 20°C, respectively. A negative specification of V_{settle}^{phy} corresponds to a downwards settling velocity.

H.4.4 Stokes

In this model, phytoplankton settling is computed using the Stokes equation and cell diameter and density, as per Equation H.19.

$$V_{sett(computed)}^{phy} = -g \times d_{phy}^2 \times \frac{(\rho_{phy} - \rho_w)}{18\mu} \quad (H.19)$$

g is acceleration due to gravity, d_{phy} and ρ_{phy} are phytoplankton cell diameter and density, respectively, and ρ_w and μ are the ambient water density and dynamic viscosity, respectively. This model is only available if phytoplankton cell density is dynamically simulated. Cell density is therefore required to be simulated as a computed variable in both cases, with supporting initial and boundary condition specifications. Cell diameter is fixed at 1×10^{-5} m.

Even though a half saturation light intensity I_K is not required to compute the settling velocity directly, it is required to compute the cell density term in Equation H.19. Cell density is computed as described in Section L.2. I_K can therefore be specified in the command to set stokes settling (referred to as I_{K-sto}), if it is not already specified in a phytoplankton constituent model light limitation function.

H.4.5 Motile

The motility settling model can only be used if internal nutrients are simulated, via deployment of the advanced phytoplankton constituent model.

In this model, phytoplankton are permitted to be motile, with the motility velocity being either a user specified value (and either upwards or downwards), or zero. This motility behaviour is governed by phytoplankton internal nutrient status and ambient environmental conditions, as follows:

- If $Q < 0.675 \times X_{N-C-max}^{phy}$ then phytoplankton is starved of nutrients and swims downwards at a rate V_{mot}^{phy}
- If $Q > 0.750 \times X_{N-C-max}^{phy}$ then phytoplankton is replete of nutrients and:
 - If local photosynthetically available radiation is greater than I_{K-mot} then phytoplankton swim up at V_{mot}^{phy}
 - If local photosynthetically available radiation is less than I_{K-mot} then phytoplankton are not motile
- If $0.675 \times X_{N-C-max}^{phy} < Q < 0.750 \times X_{N-C-max}^{phy}$ then phytoplankton are not motile

V_{mot}^{phy} is the user specified motility velocity where a negative value is treated as a downwards motility, Q is the instantaneous ratio of phytoplankton internal nitrogen to carbon computed by the WQ Module (N/C, not R_{IN-IP}^{phy}), $X_{N-C-max}^{phy}$ is the maximum internal nitrogen to carbon concentration ratio either user specified (or default) in the advanced constituent model and I_{K-mot} is the half saturation constant for light limitation of growth. A value of I_{K-mot} specified in the settling model will be ignored if it has been specified in the light limitation model.

Overriding all of the above is the condition that if local photosynthetically available radiation is greater than 95% of the water surface value, motility is set to zero as phytoplankton are considered to already be at the surface of the model domain.



I Processes: phyto limitation

I.1 General

Several functions are available within the WQ Module that allow for modification of computed phytoplankton rates in response to environmental conditions. These functions were mentioned in passing in previous Appendices and are called limitation functions because they describe how temperature, nitrogen, phosphorus, silicate, light and salinity potentially limit phytoplankton rates. Their computed values are always dimensionless and between zero and one, and are applied multiplicatively to modify initially computed rates. Limitation functions of zero completely shut off initially computed rates, and conversely, limitation functions of one do not affect these rates whatsoever. Limitation functions that are valued between zero and one linearly affect computed rates as per Equation H.2.

The key principle of limitation functions is that they provide a quantitative comparison of phytoplanktonic rate requirements with ambient conditions, and then modify phytoplankton behaviour accordingly. For example, an initially computed R_{prod}^{phy} may make a productivity demand on ambient nitrogen that exceeds instantaneous nitrogen availability. In this case, primary production will need to be reduced to reflect this nitrogen scarcity. This is affected via the multiplicative application to the initial primary productivity rate of a (computed) nitrogen limitation L_{nit}^{phy} that is less than one. A similar principle applies to temperature, phosphorus, silicate, light and salinity limitation functions: they modify computed phytoplanktonic rates based on a relative assessment of these rates to instantaneous ambient environmental conditions.

There are multiple limitation functions available within the WQ Module for each of temperature, nitrogen, phosphorus, silicate, light and salinity. These are described below.

I.2 Temperature

Temperature limitation is often considered a key influencer of phytoplankton dynamics. The WQ Module offers the following temperature limitation functions.

I.2.1 None

This model includes no temperature limitation to the computed primary productivity rate. The temperature limitation is set to 1.0 for all temperatures.

I.2.2 Standard

This is a generic yet customisable temperature limitation function. It comprises three piecewise continuous sub functions:

$$L_T^{phy} = \begin{cases} [\theta_{prod}^{phy}]^{(T-20)} & T \leq T_{std}^{phy} \\ f(T_{opt}^{phy}, T_{std}^{phy}, T_{max}^{phy}) & T_{std}^{phy} < T \leq T_{max}^{phy} \\ 0 & T_{max}^{phy} < T \end{cases} \quad (I.1)$$

θ_{prod}^{phy} is the temperature coefficient for primary productivity, f is a sub function of T_{opt}^{phy} , T_{std}^{phy} and T_{max}^{phy} , which are the optimal, standard and maximum water temperatures respectively, and T is ambient water temperature.

The function f comprises a two stage algorithm:

- **Stage 1.** Preprocess T_{opt}^{phy} , T_{std}^{phy} and T_{max}^{phy} in a once-off iterative calculation to generate a secondary suite of parameters that are then used in Stage 2 computations
- **Stage 2.** Use ambient environmental conditions, θ_{prod}^{phy} , T_{std}^{phy} and the parameters generated in Stage 1 to compute the temperature limitation function at every water quality timestep and computational cell throughout a simulation

Stage 1 The intent of Stage 1 is to use T_{opt}^{phy} , T_{std}^{phy} and T_{max}^{phy} to iteratively compute three parameters aTn , bTn and kTn that describe a curve fitting of L_T^{phy} between T_{std}^{phy} and T_{max}^{phy} (i.e. function f in Equation I.1). The conditions for this curve fitting ensure that L_T^{phy} is piecewise continuous:

$$L_T^{phy} = \begin{cases} [\theta_{prod}^{phy}]^{(T-20)} & T = T_{std}^{phy} \\ 0 & T = T_{max}^{phy} \end{cases} \quad (I.2)$$

To do so, the WQ Module uses Equation I.3 to compute the intermediate quantity G by iterating on kTn , with the kTn seed set to 6.0.

$$G = \left(kTn \times [\theta_{prod}^{phy}]^{(kTn \times T_{opt}^{phy})} \times [\theta_{prod}^{phy}]^{(T_{max}^{phy}-20.0)} - \dots \right. \\ \left. \left([\theta_{prod}^{phy}]^{(T_{opt}^{phy}-20.0)} \times \left([\theta_{prod}^{phy}]^{(kTn \times T_{max}^{phy})} - [\theta_{prod}^{phy}]^{(kTn \times T_{std}^{phy})} \right) \right) \right) \quad (I.3)$$

The iteration target is $|G| \leq 0.5$. If this target is not met on a given iteration, a new value of kTn is computed as per Equation I.4.

$$kTn = kTn - \frac{G}{\nabla G} \quad (I.4)$$

∇G is computed as per Equation I.5.

$$\nabla G = \left(\left([\theta_{prod}^{phy}]^{(kTn \times T_{opt}^{phy})} \times [\theta_{prod}^{phy}]^{(T_{max}^{phy}-20.0)} \right) \times \left(1.0 + kTn \times T_{opt}^{phy} \times \ln(\theta_{prod}^{phy}) \right) - \dots \right. \\ \left. \left([\theta_{prod}^{phy}]^{(T_{opt}^{phy}-20.0)} \times \ln(\theta_{prod}^{phy}) \times \left(T_{max}^{phy} \times [\theta_{prod}^{phy}]^{(kTn \times T_{max}^{phy})} - T_{std}^{phy} \times [\theta_{prod}^{phy}]^{(kTn \times T_{std}^{phy})} \right) \right) \right) \quad (I.5)$$

Once the iteration target is met (i.e. $|G| \leq 0.5$), the final value of kTn is used to compute aTn and bTn as per Equation I.6.

$$aTn = \frac{-\ln \left(\frac{[\theta_{prod}^{phy}]^{(T_{opt}^{phy}-20)}}{kTn \times [\theta_{prod}^{phy}]^{(kTn \times T_{opt}^{phy})}} \right)}{kTn \times \ln(\theta_{prod}^{phy})} \quad (I.6)$$

$$bTn = [\theta_{prod}^{phy}]^{kTn \times (T_{std}^{phy} - aTn)}$$

All of aTn , bTn and kTn are fixed at the end of Stage 1 for repeated use in Stage 2. and used in Stage 2 at every timestep and model cell to compute L_T^{phy} in the water temperature range between T_{std}^{phy} and T_{max}^{phy} .

Stage 2 The intent of Stage 2 is to use aTn , bTn and kTn to describe a curve for L_T^{phy} between T_{std}^{phy} and T_{max}^{phy} . This curve is computed as per Equation I.7.

$$L_T^{phy} = [\theta_{prod}^{phy}]^{(T-20)} - [\theta_{prod}^{phy}]^{kTn \times (T-aTn)} + bTn \quad (I.7)$$

The complete piecewise continuous function for the generic temperature limitation function L_T^{phy} is provided in Equation I.8.

$$L_T^{phy} = \begin{cases} [\theta_{prod}^{phy}]^{(T-20)} & T \leq T_{std}^{phy} \\ [\theta_{prod}^{phy}]^{(T-20)} - [\theta_{prod}^{phy}]^{kTn \times (T-aTn)} + bTn & T_{std}^{phy} < T \leq T_{max}^{phy} \\ 0 & T_{max}^{phy} < T \end{cases} \quad (I.8)$$

Depending on the user specification of T_{std} and T_{opt} , this limitation function can have a value greater than 1.0. This is acceptable, and can be interpreted as temperature effects actively increasing phytoplankton growth. L_T^{phy} is the only limitation function (other than limitation functions that are applied to enhance respiration due to salinity - see Section I.7.2.2, Section I.7.3.2 and Section I.7.4.2) that can vary outside the range 0.0 to 1.0.

The form of L_T^{phy} with varying T depends on three user specified (or default) temperatures and their derived quantities aTn , bTn and kTn . As such, the following two figures present L_T^{phy} varying with T and at constant $T_{max}^{phy} = 25^\circ\text{C}$, with the following conditions:

- Figure I.1:
 - Line 1: T_{std}^{phy} held constant at 10°C , with the slider varying T_{opt}^{phy}
 - Line 2: T_{std}^{phy} held constant at 18°C , with the slider varying T_{opt}^{phy}
- Figure I.2:
 - Line 1: T_{opt}^{phy} held constant at 10°C , with the slider varying T_{std}^{phy}
 - Line 2: T_{opt}^{phy} held constant at 18°C , with the slider varying T_{std}^{phy}

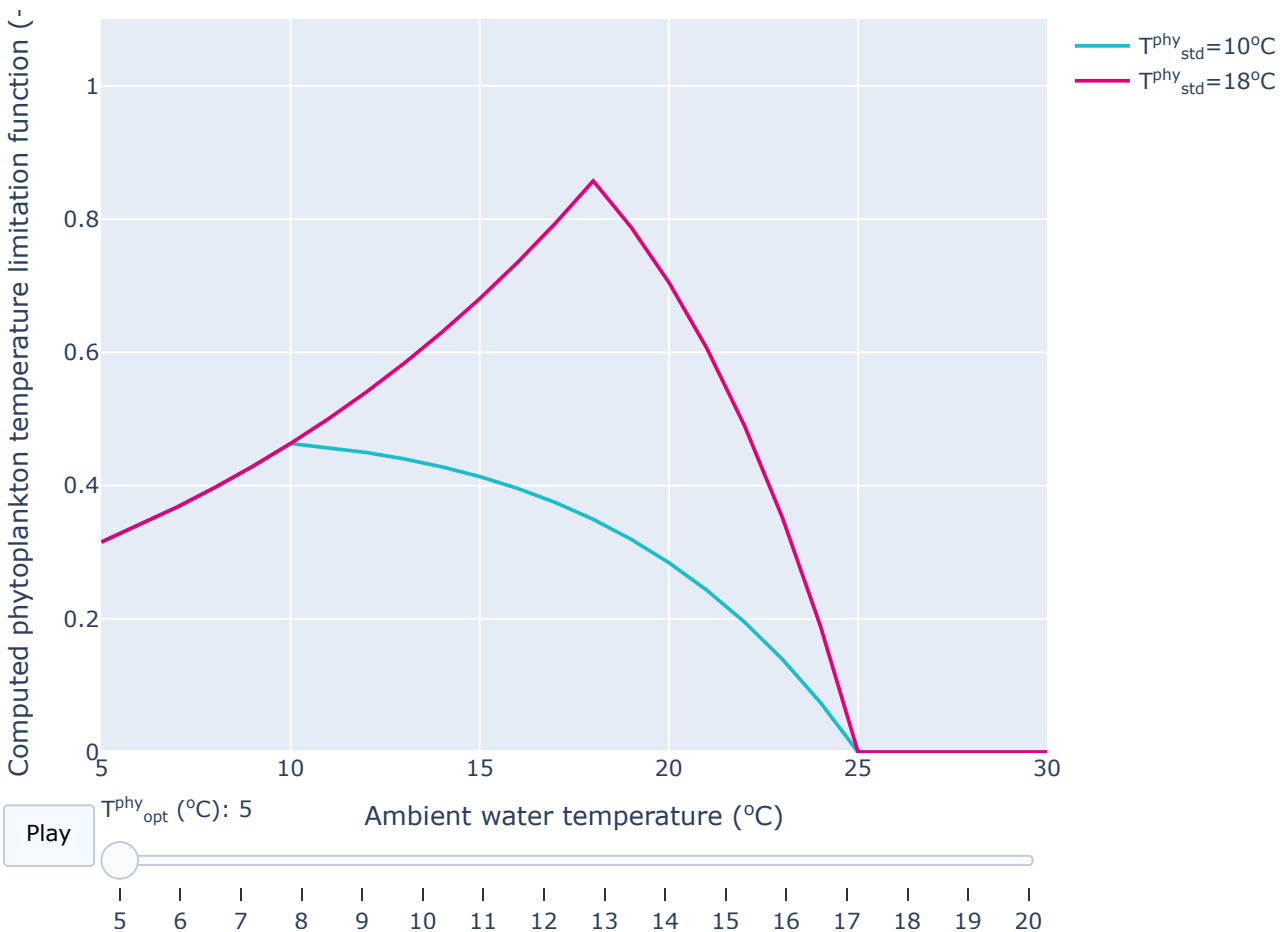


Figure I.1: Move the slider to see the effect of changing T_{opt}^{phy} on the computed temperature limitation function

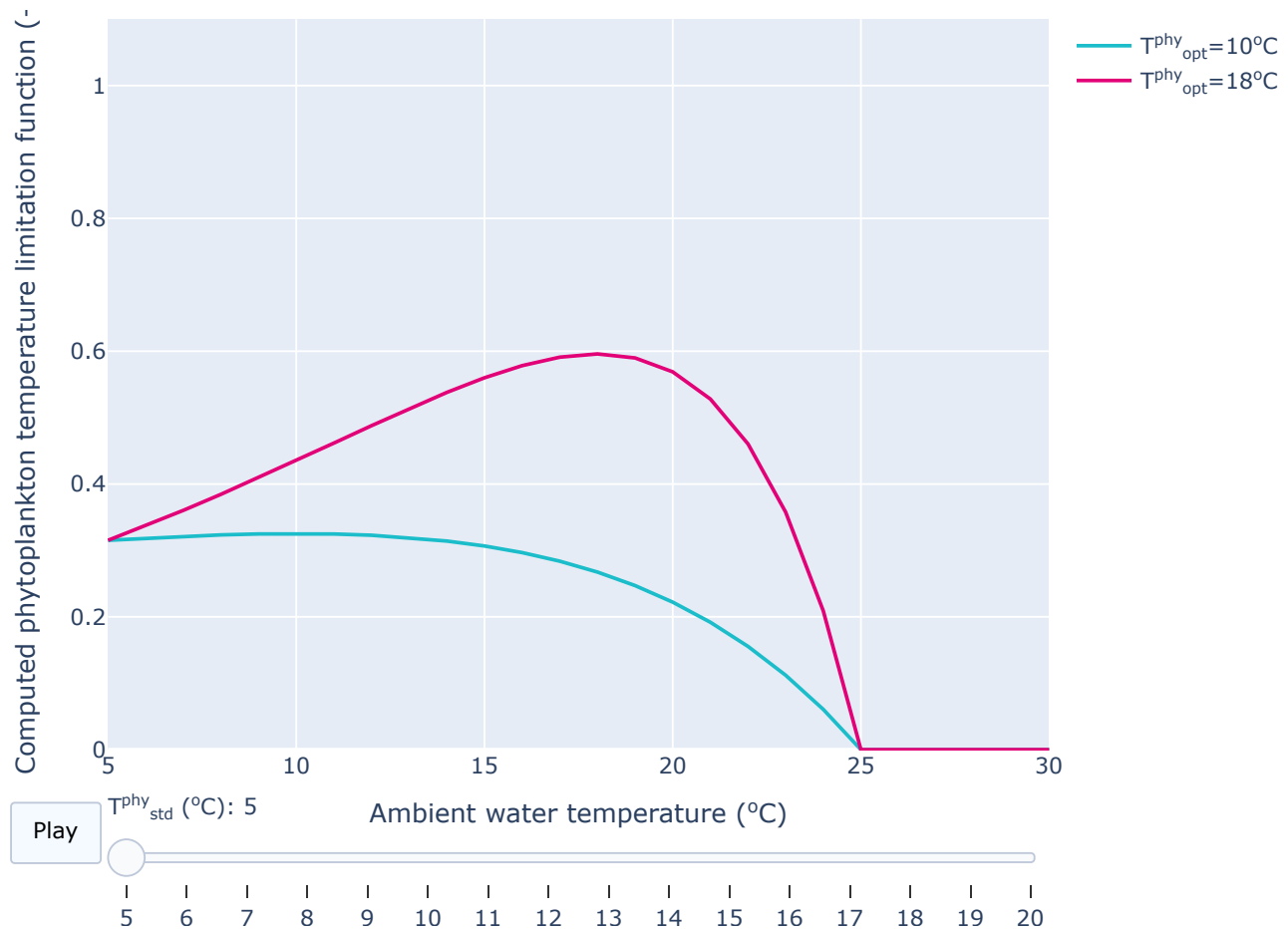


Figure I.2: Move the slider to see the effect of changing T_{std}^{phy} on the computed temperature limitation function

The WQ log file reports the computed temperature limitation function for each phytoplankton group as columnar data. Users can copy and paste these data into plotting software (such as Microsoft Excel) to view each temperature limitation function and therefore ensure that its form is as intended.

I.3 Nitrogen

Nitrogen offers two limitation functions, one for each of the basic and advanced phytoplankton constituent models. These are described separately following. If nitrogen fixing is implemented for a particular phytoplankton group, then the calculations following are not implemented and L_{nit}^{phy} is set to one.

I.3.1 Basic phytoplankton constituent model

If internal phytoplankton nutrients are not simulated dynamically, Equation I.9 is used to compute L_{nit}^{phy} .

$$L_{nit}^{phy} = \frac{([N]_{avail} - [N]_{min}^{phy})}{([N]_{avail} - [N]_{min}^{phy}) + K_{lim-N}^{phy}} \quad (I.9)$$

$[N]_{avail}$ is the available ambient nitrogen pool on which phytoplankton can draw for primary productivity, and is the sum of inorganic (ammonium and nitrate) nitrogen. $[N]_{min}^{phy}$ is the nitrogen concentration below which phytoplankton is no longer permitted to uptake nitrogen. K_{lim-N}^{phy} is the half saturation nitrogen concentration for phytoplankton uptake.

All these parameters are considered by the WQ Module to be combined quantities, i.e. they are not specific to any particular nitrogen species, but rather, to nitrogen-N concentrations across all species uptaken. In the case of the basic phytoplankton constituent model, this is simply the sum of ammonium-N and nitrate-N concentrations.

Equation I.9 has that when K_{lim-N}^{phy} is equal to the difference between ambient nitrogen concentration and $[N]_{min}^{phy}$, i.e. when

$$K_{lim-N}^{phy} = [N]_{avail} - [N]_{min}^{phy} \quad (I.10)$$

then $L_{nit}^{phy} = 0.5$. The form of L_{nit}^{phy} with varying $[N]_{min}^{phy}$ and K_{lim-N}^{phy} is provided in Figure I.3, for constant $[N]_{avail} = 1.0$ mg/L.

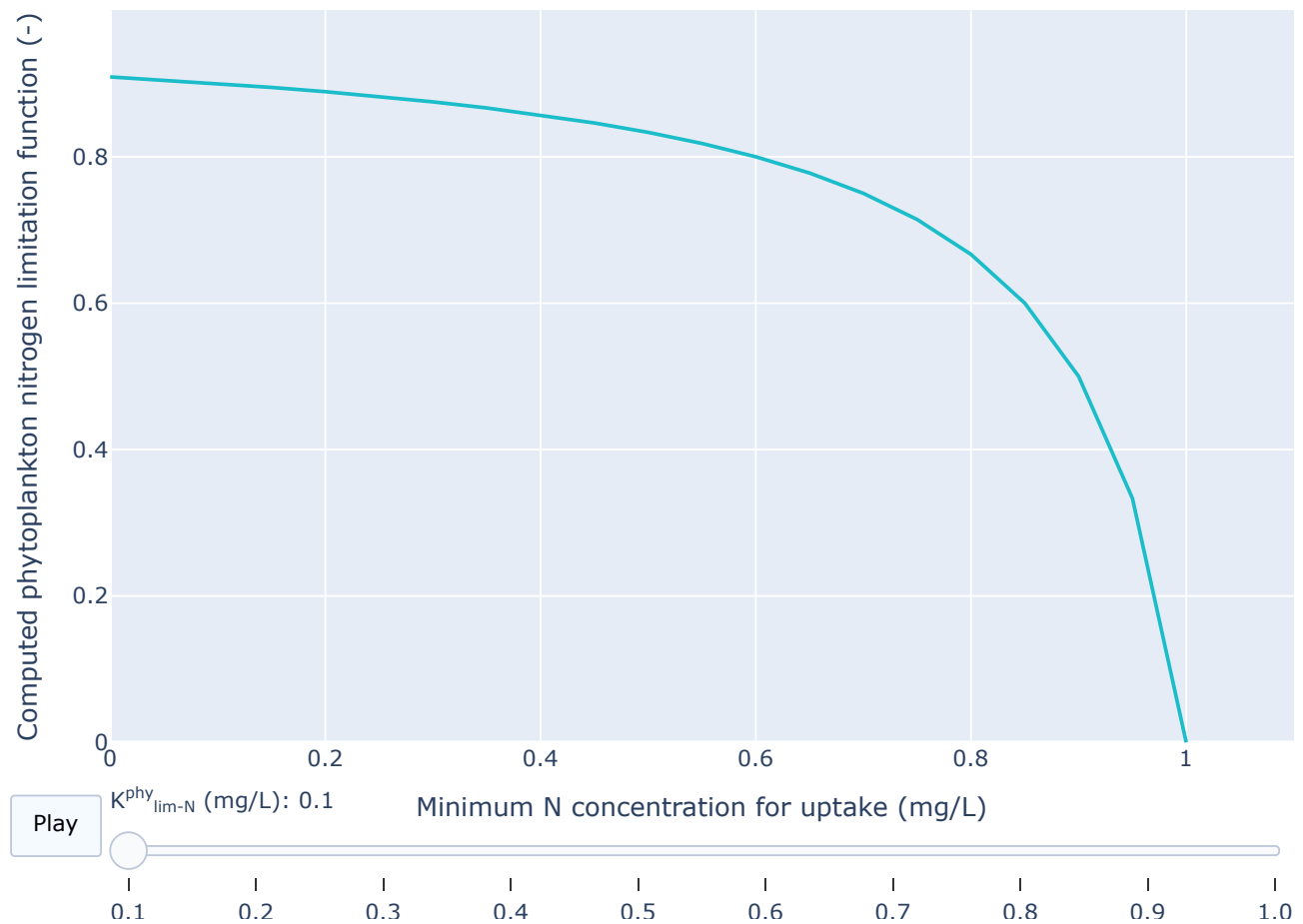


Figure I.3: Move the slider to see the effect of changing K_{lim-N}^{phy} on the computed nitrogen limitation function

The parameter K_{lim-N}^{phy} is the same as that specified in the computation of the the fraction of ammonium that is taken up with primary production (Section J.2.1) in the basic phytoplankton constituent model (Equation J.3). As such its setting should be considered in terms of its impacts on both nitrogen limitation and uptake processes.

I.3.2 Advanced phytoplankton constituent model

If internal phytoplankton nutrients are simulated dynamically, and phytoplankton concentrations are greater than the specified (or default) minimum, then Equation I.11 is used to compute L_{nit}^{phy} .

$$L_{nit}^{phy} = \frac{X_{N-C-max}^{phy} \times \left(1.0 - \frac{X_{N-C-min}^{phy} \times [PHY]}{[IN]}\right)}{X_{N-C-max}^{phy} - X_{N-C-min}^{phy}} \quad (I.11)$$

$X_{N-C-min}^{phy}$ and $X_{N-C-max}^{phy}$ are the specified (or default) minimum and maximum internal nitrogen to Chl *a* (or carbon if using mmm units) ratios, respectively and $[PHY]$ and $[IN]$ are the current internal Chl *a* (or carbon) and nitrogen concentrations in the computational cell being considered, respectively. Substituting the definition for the minimum nitrogen to Chl *a* (or carbon) ratio $X_{N-C-min}^{phy} = [IN]_{min} / [PHY]$ (where $[PHY]$ is in either mg/L or mmm units) into Equation I.11 and rearranging, reveals the form of L_{nit}^{phy} as per Equation I.12.

$$L_{nit}^{phy} = \frac{X_{N-C-max}^{phy} \times \left(1.0 - \frac{[IN]_{min}}{[IN]}\right)}{X_{N-C-max}^{phy} - X_{N-C-min}^{phy}} \quad (I.12)$$

$[IN]_{min}$ is the minimum internal nitrogen concentration corresponding to the current phytoplankton group $[PHY]$. Equation I.12 demonstrates that:

- If an internal nitrogen concentration is equal to $[IN]_{min}$, then L_{nit}^{phy} is zero. This means that no internal nitrogen is available for primary production in the current timestep and that nitrogen is therefore completely preventing growth
- If an internal nitrogen concentration is equal to $[IN]_{max}$, then L_{nit}^{phy} is one. This means that maximum internal nitrogen is available for primary production in the current timestep and that nitrogen is therefore placing no limit on growth

If internal phytoplankton nutrients are simulated dynamically, and phytoplankton concentration is less than the specified (or default) minimum, then phytoplankton will look to external (i.e. ambient water column) nitrogen pools to support primary productivity. The associated limitation function is therefore computed in the same manner as Equation I.9 in Section I.3.1. If this is the case, then the parameters K_{lim-N}^{phy} and $[N]_{min}^{phy}$ are used.

This same parameter is also used in the computation of the nitrogen that is taken up with primary production (Section J.2.2) in the advanced phytoplankton constituent model (Equation J.4). As such its setting should be considered in terms of its impacts on both nitrogen limitation and uptake processes in the advanced phytoplankton constituent model.

I.4 Phosphorus

Phosphorus offers two limitation functions, one for each of the basic and advanced phytoplankton constituent models. These are described separately following.

I.4.1 Basic phytoplankton constituent model

If internal phytoplankton nutrients are not dynamically simulated, Equation I.13 is used to compute L_{phs}^{phy} .

$$L_{phs}^{phy} = \frac{([P]_{avail} - [P]_{min}^{phy})}{([P]_{avail} - [P]_{min}^{phy}) + K_{lim-P}^{phy}} \quad (I.13)$$

$[P]_{avail}$ is the available phosphorus pool on which phytoplankton can draw for primary productivity, and is simply FRP. $[P]_{min}^{phy}$ is the phosphorus concentration below which phytoplankton no longer is permitted to uptake phosphorus. K_{lim-P}^{phy} is the half saturation phosphorus concentration for phytoplankton uptake.

Equation I.13 has that when K_{lim-P}^{phy} is equal to the difference between ambient phosphorus concentration and $[P]_{min}^{phy}$, i.e. when

$$K_{lim-P}^{phy} = [P]_{avail} - [P]_{min}^{phy} \quad (I.14)$$

then $L_{phs}^{phy} = 0.5$. The form of L_{phs}^{phy} with varying $[P]_{min}^{phy}$ and K_{lim-P}^{phy} is provided in Figure I.4, for constant $[P]_{avail} = 1.0$ mg/L.

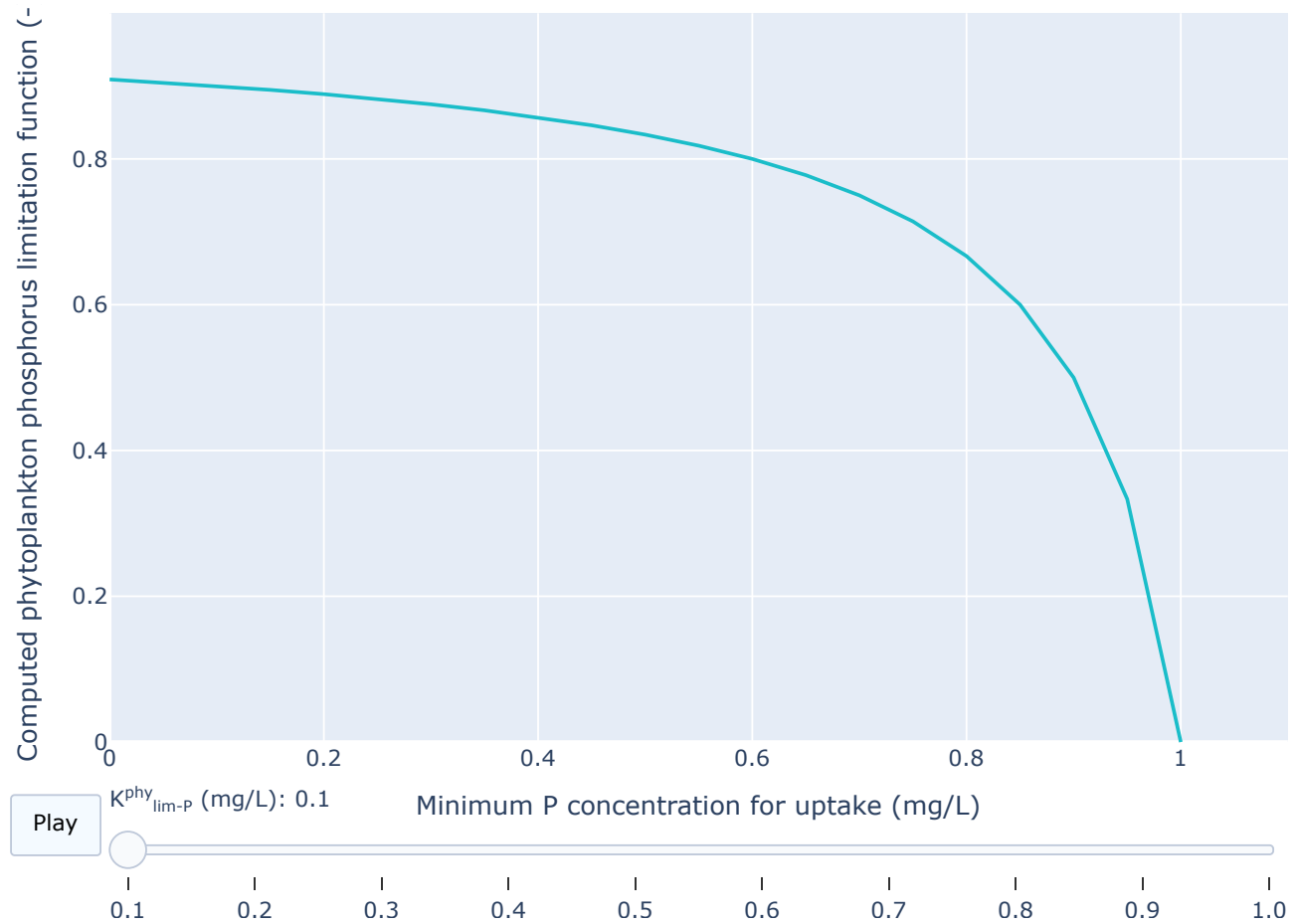


Figure I.4: Move the slider to see the effect of changing K_{lim-P}^{phy} on the computed phosphorus limitation function

1.4.2 Advanced phytoplankton constituent model

If internal phytoplankton nutrients are simulated dynamically, and phytoplankton concentrations are greater than the specified (or default) minimum, then Equation I.15 is used to compute L_{phs}^{phy} .

$$L_{phs}^{phy} = \frac{X_{P-C-max}^{phy} \times \left(1.0 - \frac{X_{P-C-min}^{phy} \times [PHY]}{[IP]}\right)}{X_{P-C-max}^{phy} - X_{P-C-min}^{phy}} \quad (I.15)$$

$X_{P-C-min}^{phy}$ and $X_{P-C-max}^{phy}$ are the specified (or default) minimum and maximum internal phosphorus to Chl *a* (or carbon if using mmm units) ratios, respectively and $[PHY]$ and $[IP]$ are the current internal Chl *a* (or carbon) and phosphorus concentrations in the computational cell being considered, respectively. Substituting the definition for the minimum phosphorus to Chl *a* (or carbon) ratio $X_{P-C-min}^{phy} = [IP]_{min} / [PHY]$ (where $[PHY]$ is in either mg/L or mmm units) into Equation I.15 and rearranging, reveals the form of L_{phs}^{phy} as per Equation I.16.

$$L_{phs}^{phy} = \frac{X_{P-C-max}^{phy} \times \left(1.0 - \frac{[IP]_{min}}{[IP]}\right)}{X_{P-C-max}^{phy} - X_{P-C-min}^{phy}} \quad (I.16)$$

$[IP]_{min}$ is the minimum internal phosphorus concentration corresponding to the current $[PHY]$. Equation I.16 demonstrates that:

- If an internal phosphorus concentration is equal to $[IP]_{min}$, then L_{phs}^{phy} is zero. This means that no internal phosphorus is available for primary production in the current timestep and that phosphorus is therefore completely preventing growth

- If an internal phosphorus concentration is equal to $[IP]_{max}$, then L_{phs}^{phy} is one. This means that maximum internal phosphorus is available for primary production in the current timestep and that phosphorus is therefore placing no limit on growth

If internal phytoplankton nutrients are simulated dynamically, and phytoplankton concentrations are less than the specified (or default) minimum, then phytoplankton will look to external (i.e. ambient water column) phosphorus pools to support primary productivity. The associated limitation function is therefore computed in the same manner as Equation I.13 in Section I.4.1. If this is the case, then the parameters K_{lim-P}^{phy} and $[P]_{min}^{phy}$ are used.

This same parameter is also used in the computation of the phosphorus that is taken up with primary production (Section J.3.2) in the advanced phytoplankton constituent model (Equation J.8). As such its setting should be considered in terms of its impacts on both phosphorus limitation and uptake processes in the advanced phytoplankton constituent model.

I.5 Silicate

Equation I.17 is used to compute L_{sil}^{phy} , if phytoplankton is configured to take up silicate. Specifying silicate limitation parameters will trigger the WQ Module to take up silicate (Section 4.7.3.5.1.6).

$$L_{sil}^{phy} = \frac{([Si] - [Si]_{min})}{([Si] - [Si]_{min}) + K_{lim-Si}^{phy}} \quad (I.17)$$

$[Si]$ is the ambient silicate concentration. $[Si]_{min}$ is the silicate concentration below which phytoplankton no longer is permitted to uptake silicate and K_{lim-Si}^{phy} is the half saturation silicate concentration for phytoplankton uptake.

K_{lim-Si}^{phy} is specified as a silicate concentration. When this concentration is equal to the difference between the relevant ambient concentration and $[Si]_{min}$, i.e. when

$$K_{lim-Si}^{phy} = [Si] - [Si]_{min} \quad (I.18)$$

then $L_{sil}^{phy} = 0.5$. The form of L_{sil}^{phy} with varying $[Si]_{min}$ and K_{lim-Si}^{phy} is provided in Figure I.5, for constant $[Si]_{avail} = 1.0$ mg/L.

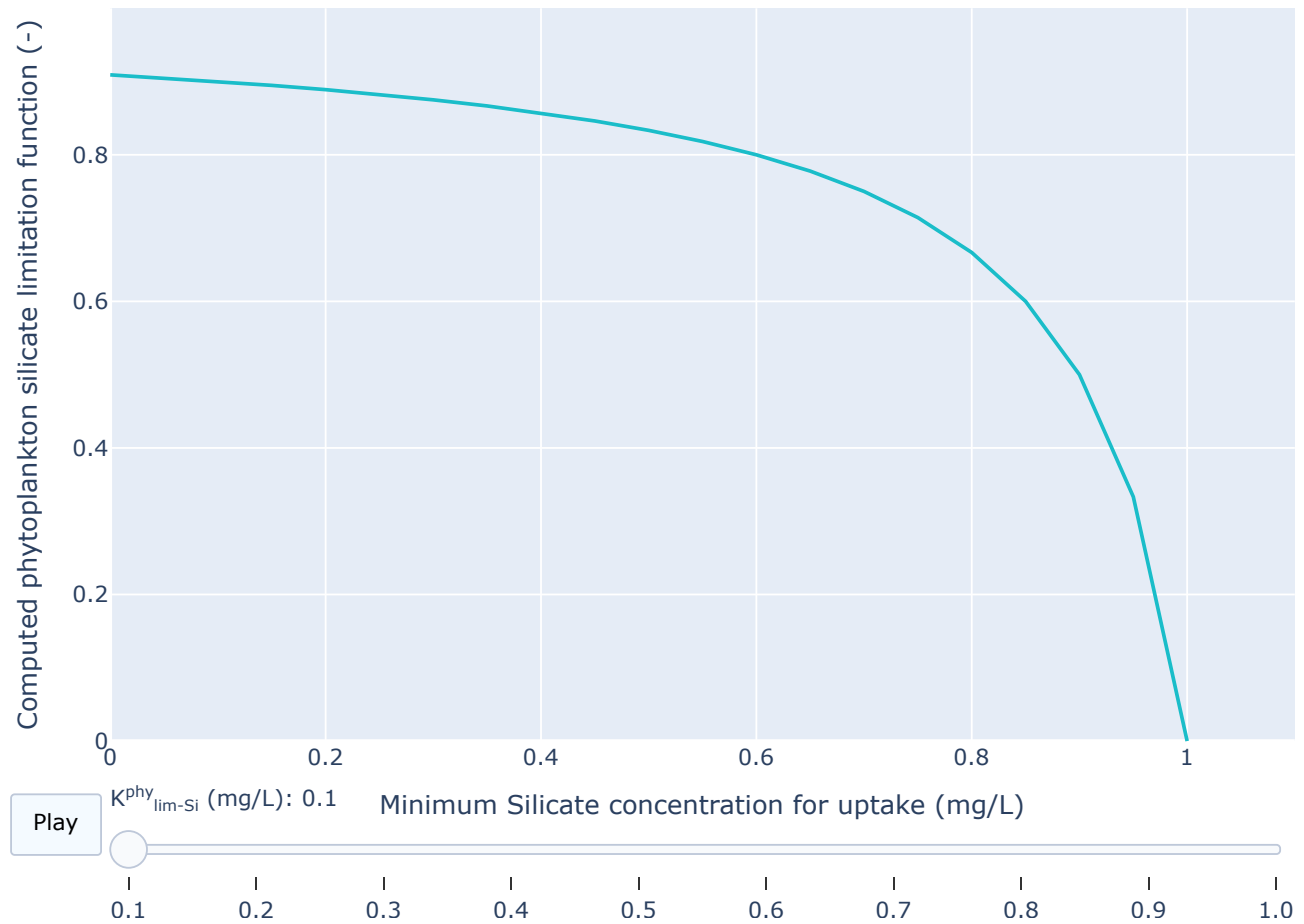


Figure I.5: Move the slider to see the effect of changing K_{lim-Si}^{phy} on the computed silicate limitation function

I.6 Light

Phytoplankton require photosynthetically active radiation (PAR) in order to affect primary productivity. The required PAR may not always be available due to a range of environmental factors and as such may limit phytoplankton growth. In addition, some phytoplankton groups may suffer photoinhibition, which is a reduction in the ability to photosynthesise as a result of damage incurred by greater levels of radiation than can be tolerated. This is also referred to as light-induced damage, and in general terms means that increasing light intensity experienced by a phytoplankton group does not translate into a monotonic increase in the light limitation function: primary productivity can decrease with increasing available light where photoinhibition occurs. A saturating light intensity I_S is specified for those models that include photoinhibition (rather than a half saturation light for limitation I_K specified for models that exclude photoinhibition) and I_S can be interpreted as the light intensity at which the limitation function has its peak, usually at a value of 1.0. Either side of this I_S light intensity, the limitation function decreases toward zero.

The WQ Module offers a number of different models that deploy combinations of these processes to estimate phytoplankton light limitation functions. These are described following.

I.6.1 Basic

This model includes phytoplankton light limitation but with no photoinhibition. Limitation is therefore purely due to insufficient light availability. The limitation function L_{light}^{phy} is computed within a model cell as per Equation I.19.

$$L_{light}^{phy} = 1.0 - \left[\int_{\frac{-PAR_b}{I_{K-bas}}}^{\infty} \left(\frac{e^{-t}}{t} \right) dt - \int_{\frac{-PAR_t}{I_{K-bas}}}^{\infty} \left(\frac{e^{-t}}{t} \right) dt \right] \times \left[\frac{1}{\max(k_{bio} \times dz, 10^{-3})} \right] \quad (I.19)$$

PAR_b and PAR_t are photosynthetically available radiation at the bottom and top faces of a model cell, respectively, I_{K-bas} is the half saturation constant for light limitation of growth, k_{bio} is the local change in light extinction coefficient due to self shading and dz is cell vertical thickness.

I.6.2 Monod

This model includes phytoplankton light limitation but with no photoinhibition, as per Monod (1950). Limitation is therefore purely due to insufficient light availability. The limitation function L_{light}^{phy} is computed within a model cell as per Equation I.20.

$$L_{light}^{phy} = \frac{\frac{PAR_c}{I_{K-mon}}}{1 + \frac{PAR_c}{I_{K-mon}}} \quad (I.20)$$

PAR_c is the photosynthetically available radiation at the centre of a model cell and I_{K-mon} is the half saturation constant for light limitation of growth. Equation I.20 has that when PAR_c is equal to I_{K-mon} , $L_{light}^{phy} = 0.5$.

I.6.3 Steele

This model includes phytoplankton light limitation with photoinhibition, as per Steele (1962). The limitation function L_{light}^{phy} is computed within a model cell as per Equation I.21.

$$L_{light}^{phy} = \frac{PAR_c}{I_{S-ste}} \times e^{\left(1.0 - \frac{PAR_c}{I_{S-ste}}\right)} \quad (I.21)$$

PAR_c is the photosynthetically available radiation at the centre of a model cell and I_{S-ste} is the saturating light intensity. Equation I.21 has that when PAR_c is equal to I_{S-ste} , $L_{light}^{phy} = 1.0$, i.e., the light intensity at which no light limitation or photoinhibition occurs. The form of Equation I.21 is presented in Figure I.6, with the abscissa spanning a typical range of instantaneous photosynthetically available radiation.

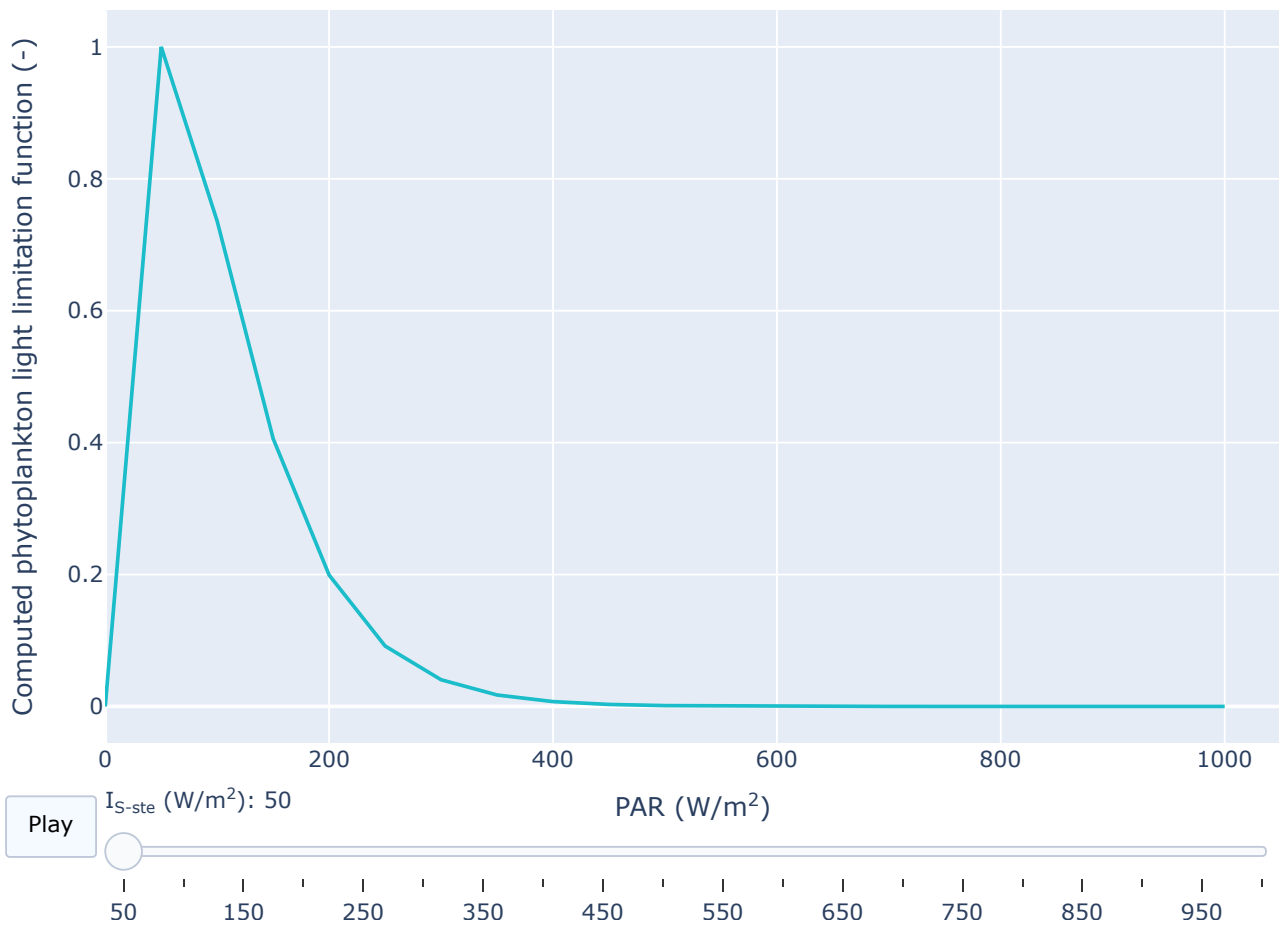


Figure I.6: Move the slider to see the effect of changing I_S on the computed light limitation function

I.6.4 Webb

This model includes phytoplankton light limitation with no photoinhibition, as per Webb (1974). The limitation function L_{light}^{phy} is computed within a model cell as per Equation I.22.

$$L_{light}^{phy} = 1.0 - e^{-\left(\frac{PAR_c}{I_{K-web}}\right)} \quad (I.22)$$

PAR_c is the photosynthetically available radiation at the centre of a model cell and I_{K-web} is the half saturation constant for light limitation of growth. The form of Equation I.22 is presented in Figure I.7, with the abscissa spanning a typical range of instantaneous photosynthetically available radiation.

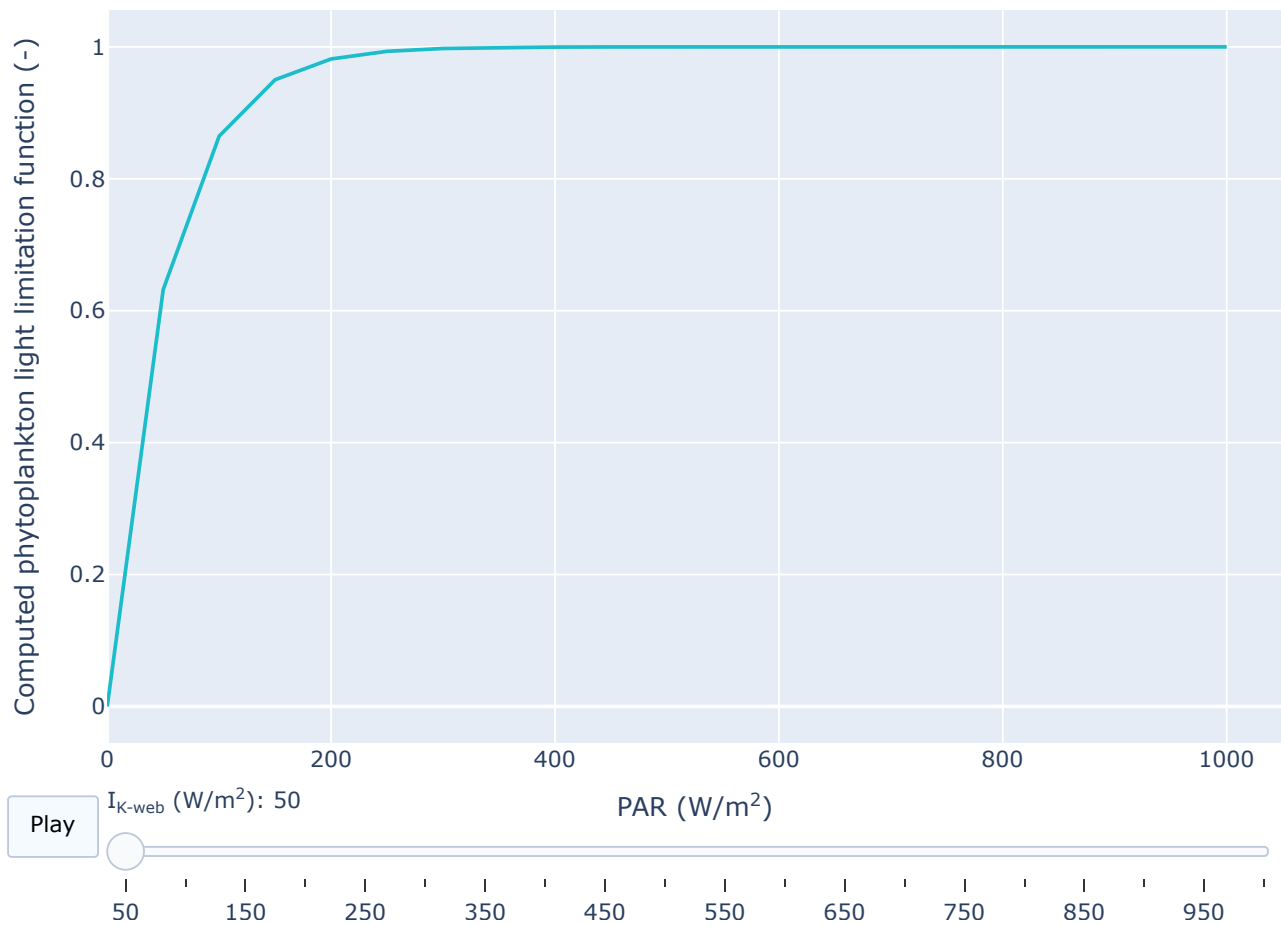


Figure I.7: Move the slider to see the effect of changing I_K on the computed light limitation function

I.6.5 Jassby

This model includes phytoplankton light limitation with no photoinhibition, as per Jassby and Platt (1976). The limitation function L_{light}^{phy} is computed within a model cell as per Equation I.23.

$$L_{light}^{phy} = \tanh\left(\frac{PAR_c}{I_{K-jas}}\right) \quad (I.23)$$

PAR_c is the photosynthetically available radiation at the centre of a model cell and I_{K-jas} is the half saturation constant for light limitation of growth. The form of Equation I.23 is presented in Figure I.8, with the abscissa spanning a typical range of instantaneous photosynthetically available radiation.

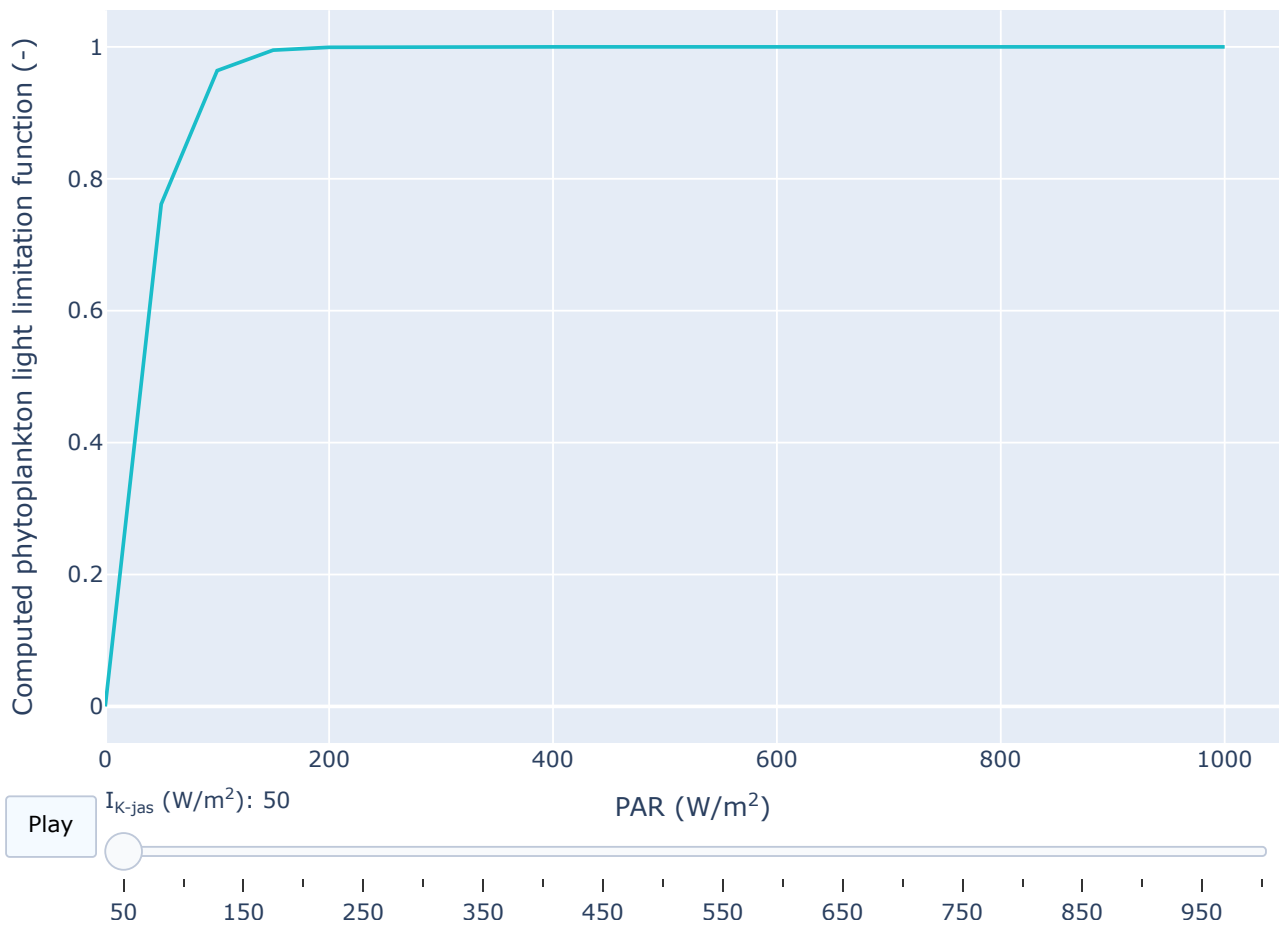


Figure I.8: Move the slider to see the effect of changing I_K on the computed light limitation function

1.6.6 Chalker

This model includes phytoplankton light limitation with no photoinhibition, as per Chalker (1980). The limitation function L_{light}^{phy} is computed within a model cell as per Equation 1.24.

$$L_{light}^{phy} = \frac{e^{1.5\left(\frac{PAR_c}{I_{K-cha}}\right)} - 1.0}{e^{1.5\left(\frac{PAR_c}{I_{K-cha}}\right)} + 0.5} \quad (1.24)$$

PAR_c is the photosynthetically available radiation at the centre of a model cell and I_{K-cha} is the half saturation constant for light limitation of growth. The form of Equation 1.24 is presented in Figure 1.9, with the abscissa spanning a typical range of instantaneous photosynthetically available radiation.

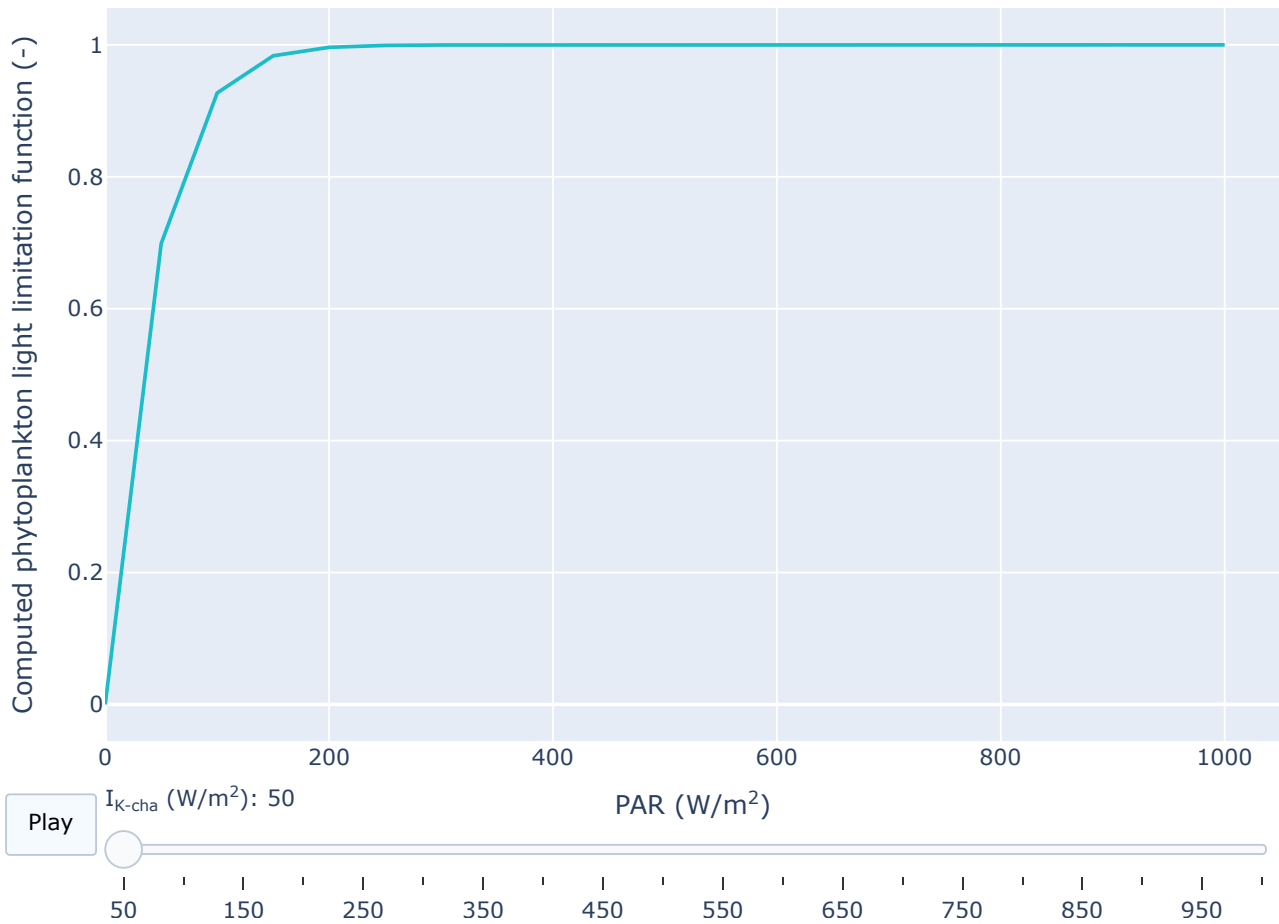


Figure I.9: Move the slider to see the effect of changing I_K on the computed light limitation function

I.6.7 Klepper

This model includes phytoplankton light limitation with photoinhibition, as per Klepper et al. (1988) and Ebenhoh et al. (1997). The limitation function L_{light}^{phy} is computed within a model cell as per Equation I.25.

$$L_{light}^{phy} = \frac{7.0 \times \left(\frac{PAR_c}{I_{S-kle}} \right)}{1.0 + 5.0 \times \left(\frac{PAR_c}{I_{S-kle}} \right) + \left(\frac{PAR_c}{I_{S-kle}} \right)^2} \quad (I.25)$$

PAR_c is the photosynthetically available radiation at the centre of a model cell and I_{S-kle} is the saturating light intensity. The form of Equation I.25 is presented in Figure I.10, with the abscissa spanning a typical range of instantaneous photosynthetically available radiation.

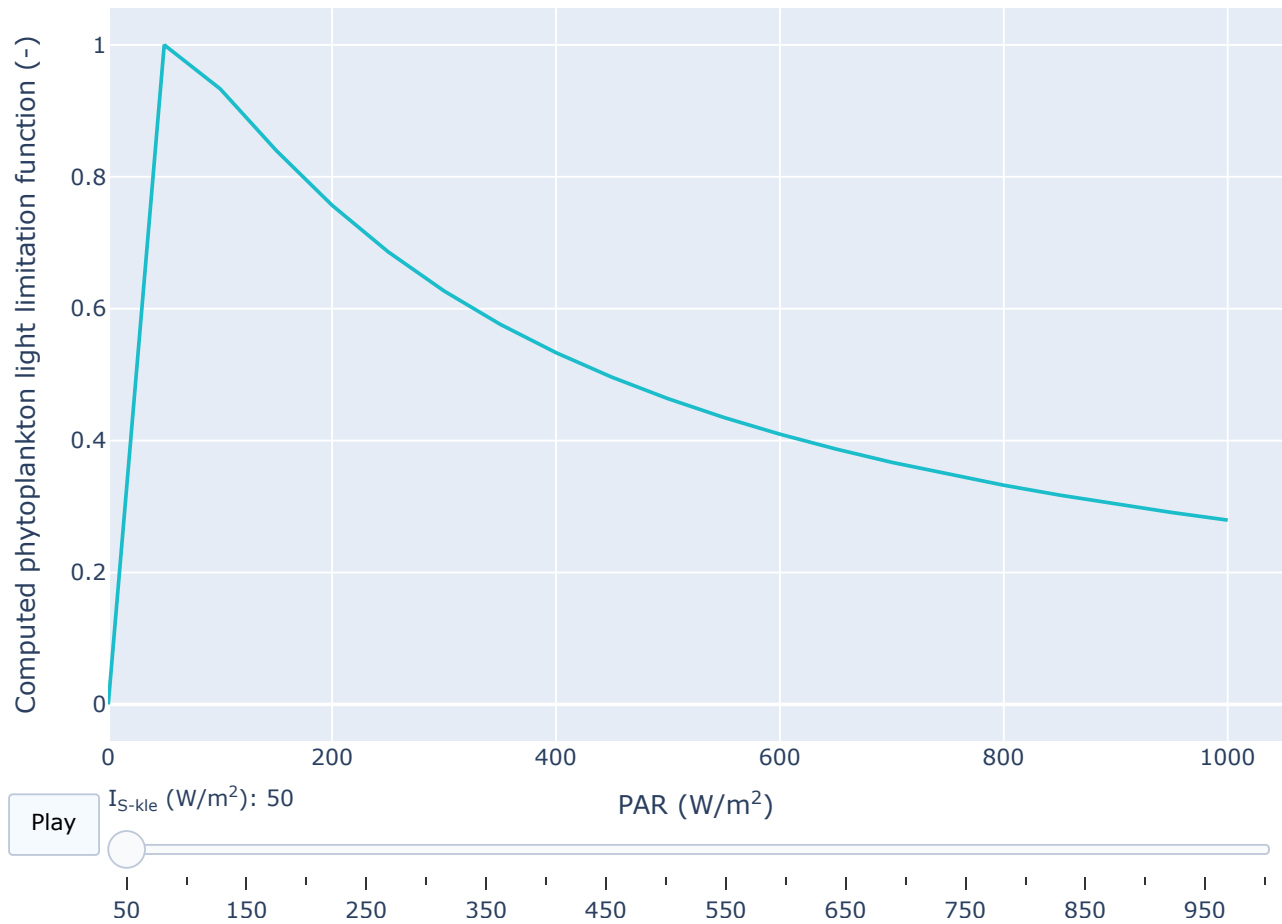


Figure I.10: Move the slider to see the effect of changing I_S on the computed light limitation function

I.6.8 Integrated

This model includes phytoplankton light limitation with photoinhibition, and is the integrated form of the Steele (1962) model provided in Equation I.21. In this form, the limitation function L_{light}^{phy} is computed within a model cell as per Equation I.26.

$$L_{light}^{phy} = \frac{e^{\left(1.0 - \frac{PAR_b}{I_{S-int}}\right)} - e^{\left(1.0 - \frac{PAR_t}{I_{S-int}}\right)}}{k_{bio} \times dz} \quad (I.26)$$

PAR_b and PAR_t are photosynthetically available radiation at the bottom and top faces of a model cell, respectively, I_{S-int} is the saturating light intensity, k_{bio} is the local change in light extinction coefficient due to self shading and dz is cell vertical thickness. In most cases, this model should produce similar results to the Steele model in Section I.6.3.

I.7 Salinity

Phytoplankton can exhibit sensitivity to salinity. Where activated, the WQ Module captures these sensitivities via multiplicative application of a salinity limitation function as either a reduction of primary productivity (Equation H.4) or an increase of respiration (Equation H.7). Application of these rates is mutually exclusive for a given phytoplankton group: limitation can be applied either to primary productivity or respiration, but not both. One way to conceptualise this is as follows:

- A salinity limitation L_{sal-pp}^{phy} applied to primary productivity is always between zero and one and will result in a reduction in primary productivity. Corresponding respiration rates will remain unaffected by salinity and therefore by Equation H.1, phytoplankton biomass should be expected to decrease as a result

- A salinity limitation L_{sal-r}^{phy} applied to respiration is always greater than one and will result in an enhancement of respiration. Corresponding primary productivity rates will remain unaffected by salinity and therefore by Equation H.1, phytoplankton biomass should be expected to decrease as a result, noting however that exudation (which is another loss term) will continue and is related to primary productivity

The salinity limitation models available within the WQ Module are described following. All can be applied to both primary productivity and respiration, other than the estuarine limitation function which is applicable only to productivity.

I.7.1 None

This model includes no salinity limitation to either of the computed primary productivity or respiration rates. The salinity limitation set to 1.0 for all salinities.

I.7.2 Freshwater

This model is typically used for phytoplankton groups that have a preference for fresh water. As such, the salinity limitation is set to 1.0 for all salinities greater than zero and up to a specified (or default) optimal salinity. The general expression for the limitation function above this optimal salinity is presented in Equation I.27, and this expression is applied to both primary productivity and respiration. Its specific applications to these two processes are described in the following subsections.

$$L_{sal-r}^{phy} = L_{sal-pp}^{phy} = \begin{cases} 1.0 & S \leq S_{opt-fresh}^{phy} \\ \left(\frac{(L_{max-fresh}^{phy} - 1.0) \times S^2 - (L_{max-fresh}^{phy} - 1.0) \times 2.0 \times S_{opt-fresh}^{phy} \times S}{(S_{max-fresh}^{phy} - S_{opt-fresh}^{phy})^2} \right) + \dots & \\ \dots \left(\frac{((L_{max-fresh}^{phy} - 1.0) \times (S_{opt-fresh}^{phy})^2)}{(S_{max-fresh}^{phy} - S_{opt-fresh}^{phy})^2} \right) + 1.0 & S_{opt-fresh}^{phy} < S \end{cases} \quad (I.27)$$

$S_{opt-fresh}^{phy}$ and $S_{max-fresh}^{phy}$ are the optimal and maximum salinities respectively, $L_{max-fresh}^{phy}$ is the value of the salinity limitation function at $S_{max-fresh}^{phy}$ and S is ambient salinity.

I.7.2.1 Primary productivity

In order to apply this limitation function to primary productivity, $L_{max-fresh}^{phy}$ is set such that

$$0.0 \leq L_{max-fresh}^{phy} \leq 1.0 \quad (I.28)$$

In this case, and with increasing salinity, the limitation function decreases from 1.0 at $S_{opt-fresh}^{phy}$ to a specified (or default) limitation function value at a specified (or default) maximum salinity. If $L_{max-fresh}^{phy}$ is not zero, then the function continues downward to zero at salinities greater than $S_{max-fresh}^{phy}$. When the function reaches zero it remains there.

The simplest application of this limitation function is to set $L_{max-fresh}^{phy}$ as zero at $S_{max-fresh}^{phy}$. This will ensure that no primary productivity occurs above a maximum salinity of $S_{max-fresh}^{phy}$ (this approach is reflected in the naming of $L_{max-fresh}^{phy}$ and $S_{max-fresh}^{phy}$). For example, if a particular phytoplankton group was known to feel the effects of salinity on primary productivity above a salinity of 5 g/L, and to entirely cease producing at salinities greater than 10 g/L, then the following would be set by the user:

- $S_{opt-fresh}^{phy} = 5.0$ g/L
- $S_{max-fresh}^{phy} = 10.0$ g/L, and

- $L_{max-fresh}^{phy} = 0.0$

Using these values initially but varying $S_{max-fresh}^{phy}$, the form of Equation I.27 is presented in Figure I.11.

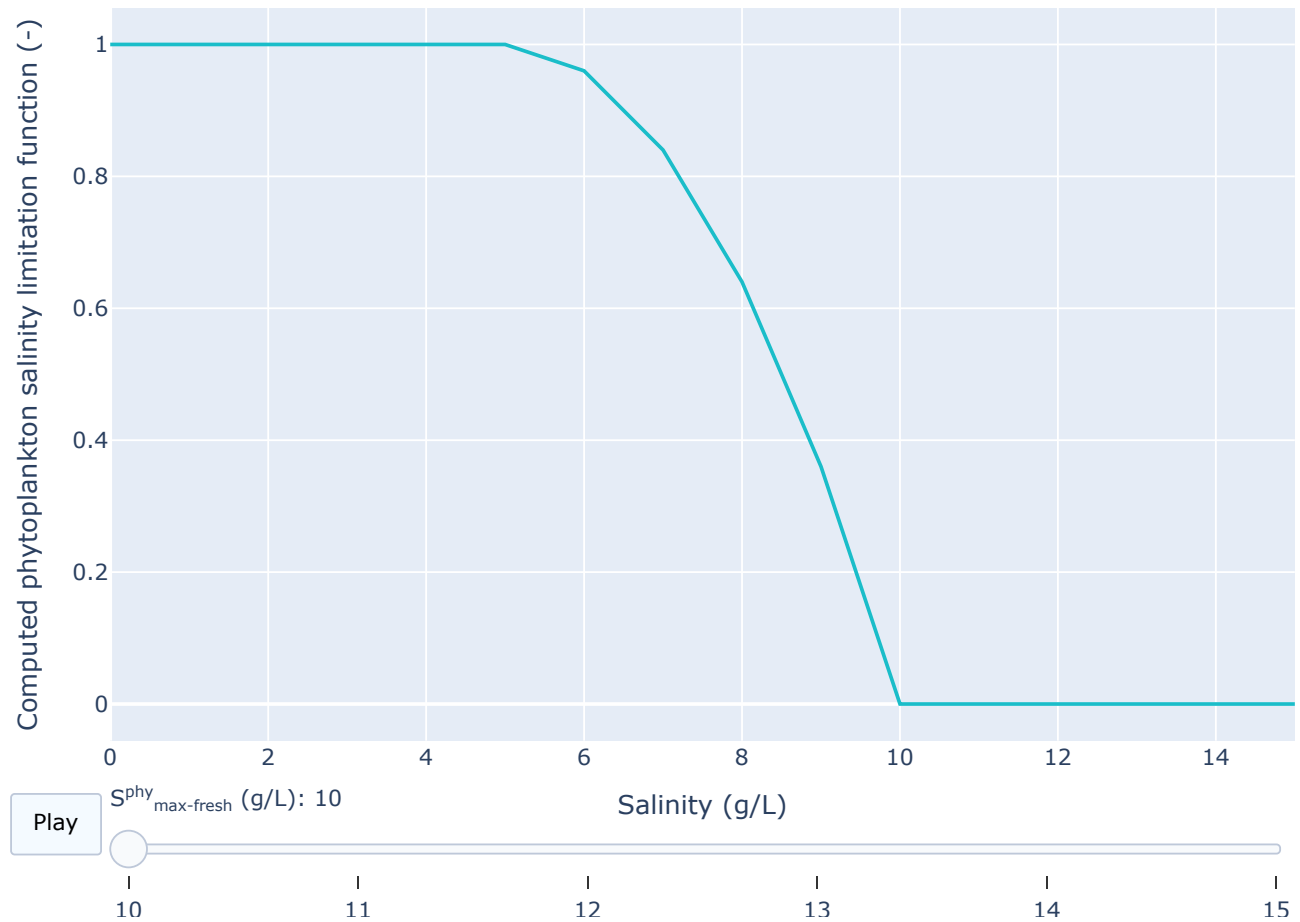


Figure I.11: Move the slider to see the effect of changing $S_{max-fresh}^{phy}$ on the computed salinity limitation function. $S_{opt-fresh}^{phy} = 5.0$ g/L and $L_{max-fresh}^{phy} = 0.0$ and are fixed

Another example is the case where $L_{max-fresh}^{phy}$ is not zero at $S_{max-fresh}^{phy}$. For example, if a particular phytoplankton group was known to feel the effects of salinity on primary productivity above a salinity of 2 g/L, and to have a 75% limitation on productivity at a salinity of 10 g/L, then the following would be set by the user:

- $S_{opt-fresh}^{phy} = 2.0$ g/L
- $S_{max-fresh}^{phy} = 10.0$ g/L, and
- $L_{max-fresh}^{phy} = 0.25$

Using these values initially, but varying $S_{max-fresh}^{phy}$, the form of Equation I.27 is presented in Figure I.12. The salinity at which the limitation function falls to zero is greater than $S_{max-fresh}^{phy}$, but is always 0.25 at $S_{max-fresh}^{phy}$.

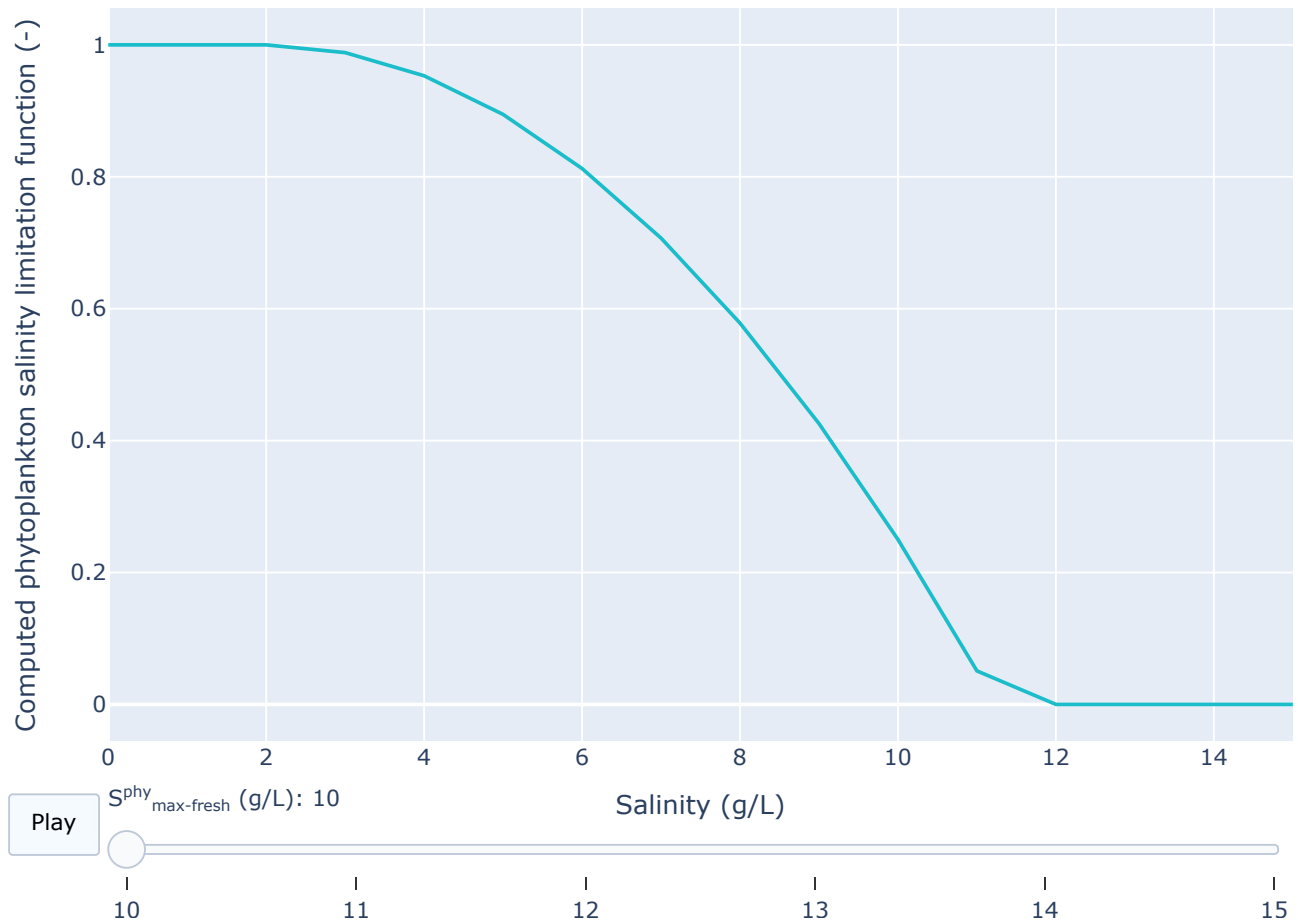


Figure I.12: Move the slider to see the effect of changing $S_{max-fresh}^{phy}$ on the computed salinity limitation function. $S_{opt-fresh}^{phy} = 2.0$ g/L and $L_{max-fresh}^{phy} = 0.25$ and are fixed

1.7.2.2 Respiration

In order to apply this limitation function to respiration, $L_{max-fresh}^{phy}$ is set such that

$$1.0 < L_{max-fresh}^{phy} \quad (I.29)$$

In this case, and with increasing salinity, the limitation function increases from 1.0 at $S_{opt-fresh}^{phy}$ to a specified (or default) limitation function value at a specified (or default) salinity. The function then increases indefinitely.

For example, if a particular phytoplankton group was known to feel the effects of salinity on respiration above a salinity of 5 g/L, such that at a salinity of 10 g/L its respiration rate doubled, then the following would be set by the user:

- $S_{opt-fresh}^{phy} = 5.0$ g/L
- $S_{max-fresh}^{phy} = 10.0$ g/L, and
- $L_{max-fresh}^{phy} = 2.0$

Using these values initially but varying $S_{max-fresh}^{phy}$, the form of Equation I.27 is presented in Figure I.13.

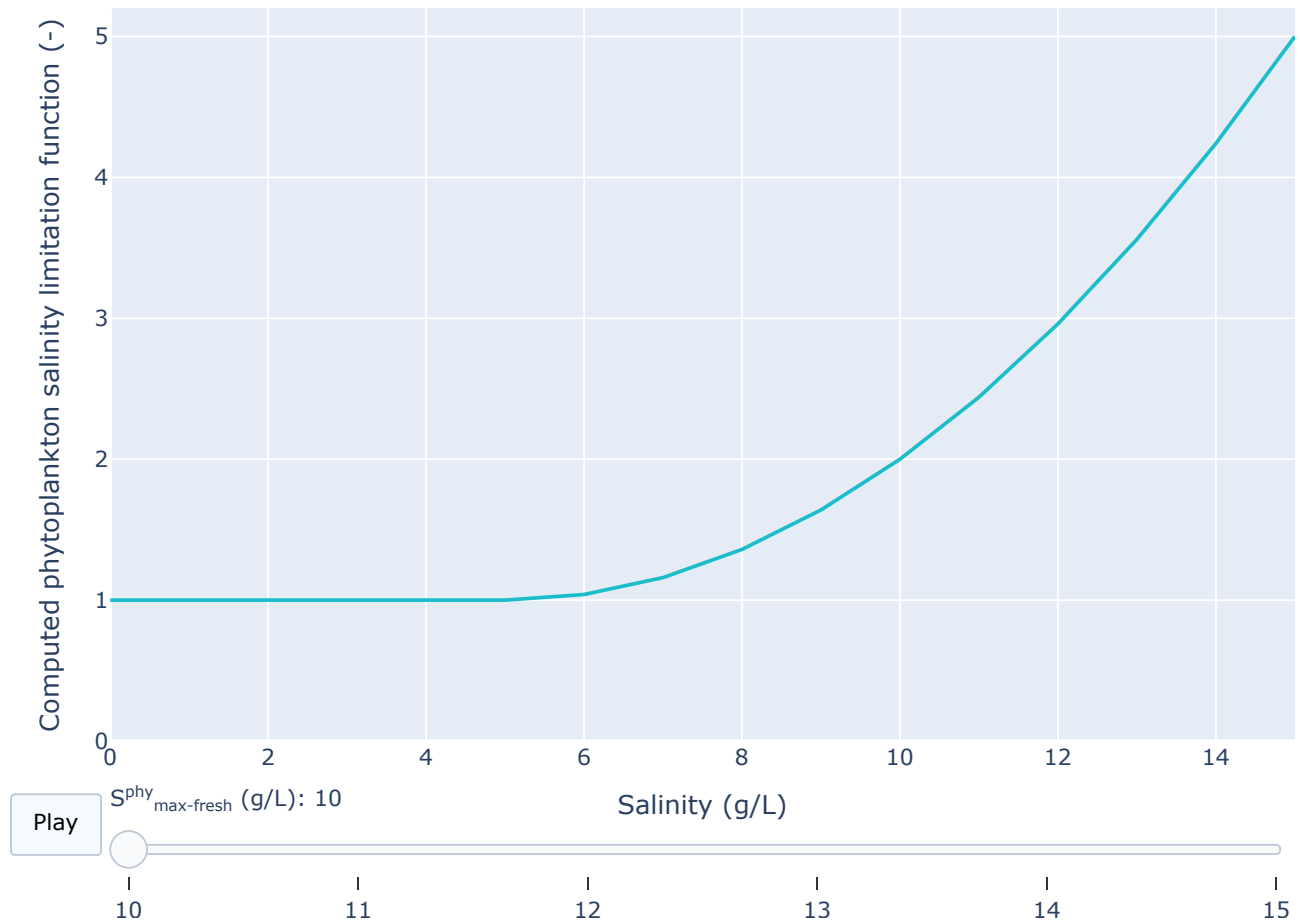


Figure I.13: Move the slider to see the effect of changing $S_{max-fresh}^{phy}$ on the computed salinity limitation function. $S_{opt-fresh}^{phy} = 5.0$ g/L and $L_{max-fresh}^{phy} = 2.0$ and are fixed

1.7.3 Marine

This model is typically used for phytoplankton groups that have a preference for marine (saline) water. As such, the salinity limitation is set to 1.0 for all salinities greater a specified (or default) optimal salinity. The general expression for the limitation function below this optimal salinity is presented in Equation 1.30, and this expression is applied to both primary productivity and respiration. Its specific applications to these two processes are described in the following subsections.

$$L_{sal-r}^{phy} = L_{sal-pp}^{phy} = \begin{cases} \left(\frac{(L_{zero-marine}^{phy} - 1.0) \times S^2}{(S_{opt-marine}^{phy})^2} \right) - \left(2.0 \times \frac{(L_{zero-marine}^{phy} - 1.0) \times S}{S_{opt-marine}^{phy}} \right) + L_{zero-marine}^{phy} & S \leq S_{opt-marine}^{phy} \\ 1.0 & S_{opt-marine}^{phy} < S \end{cases} \quad (1.30)$$

$S_{opt-marine}^{phy}$ is the optimal salinity, $L_{zero-marine}^{phy}$ is the value of the salinity limitation function at zero salinity and S is ambient salinity.

1.7.3.1 Primary productivity

In order to apply this limitation function to primary productivity, $L_{zero-marine}^{phy}$ is set such that

$$0.0 \leq L_{zero-marine}^{phy} \leq 1.0 \quad (I.31)$$

In this case, and with decreasing salinity, the limitation function decreases from 1.0 at $S_{opt-marine}^{phy}$ to a specified (or default) limitation function value at zero salinity, $L_{zero-marine}^{phy}$.

The simplest application of this limitation function is to set $L_{zero-marine}^{phy}$ to zero. This will ensure that no primary productivity occurs at zero salinity. For example, if a particular phytoplankton group was known to feel the effects of salinity on primary productivity below a salinity of 20 g/L, and to entirely cease producing at salinities of 0 g/L, then the following would be set by the user:

- $S_{opt-marine}^{phy} = 20.0$ g/L, and
- $L_{zero-marine}^{phy} = 0.0$

Using these values initially but varying $S_{opt-marine}^{phy}$, the form of Equation I.30 is presented in Figure I.14.

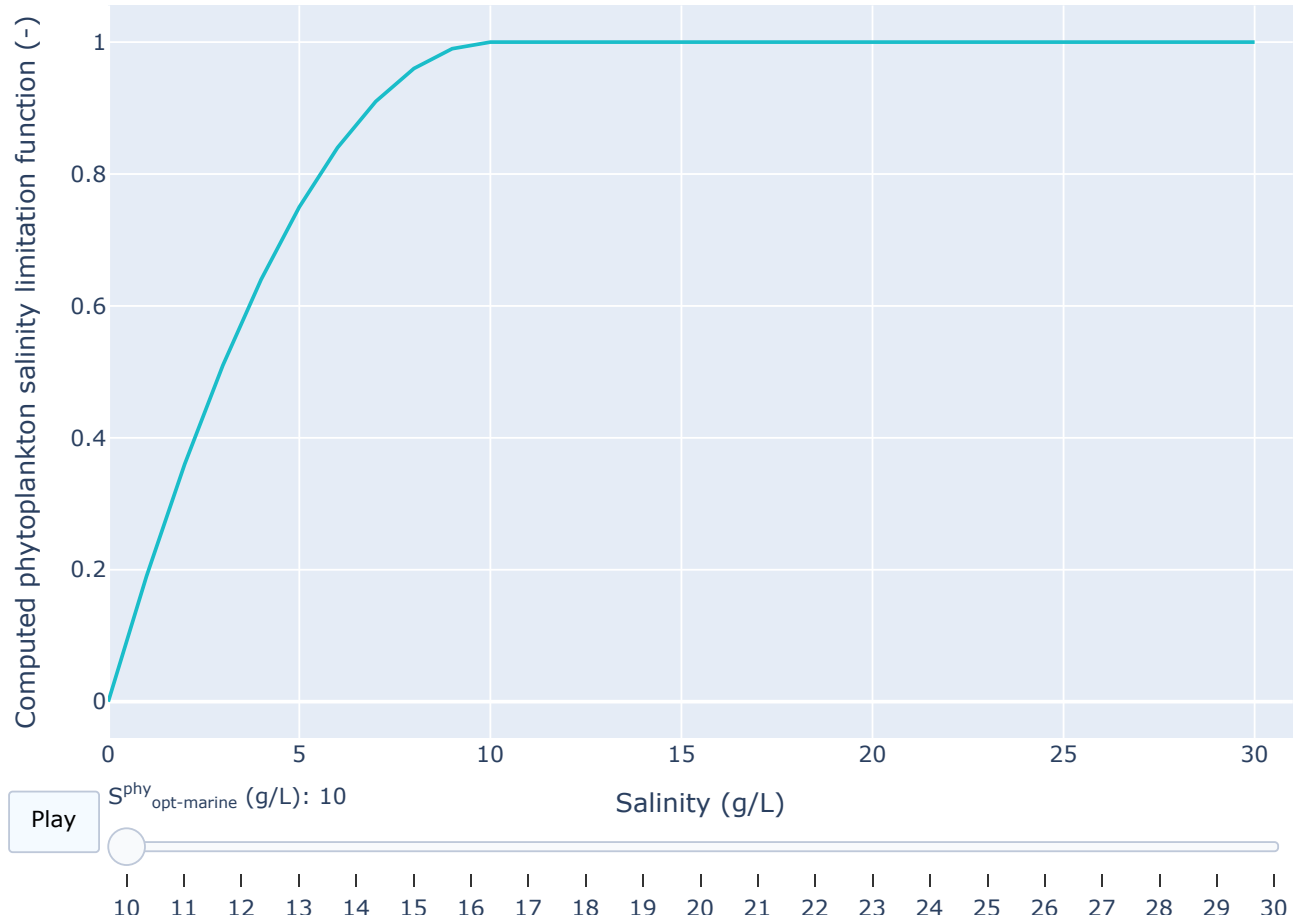


Figure I.14: Move the slider to see the effect of changing $S_{opt-marine}^{phy}$ on the computed salinity limitation function. $L_{zero-marine}^{phy} = 0.0$ and is fixed

Another example is the case where $L_{zero-marine}^{phy}$ is not zero. For example, if a particular phytoplankton group was known to feel the effects of salinity on primary productivity below a salinity of 10 g/L, and to have a 75% limitation on productivity at a salinity of 0 g/L (i.e. still produce in completely fresh water), then the following would be set by the user:

- $S_{opt-marine}^{phy} = 10.0$ g/L, and
- $L_{zero-marine}^{phy} = 0.25$

Using these values initially, but varying $S_{zero-marine}^{phy}$, the form of Equation I.30 is presented in Figure I.15.

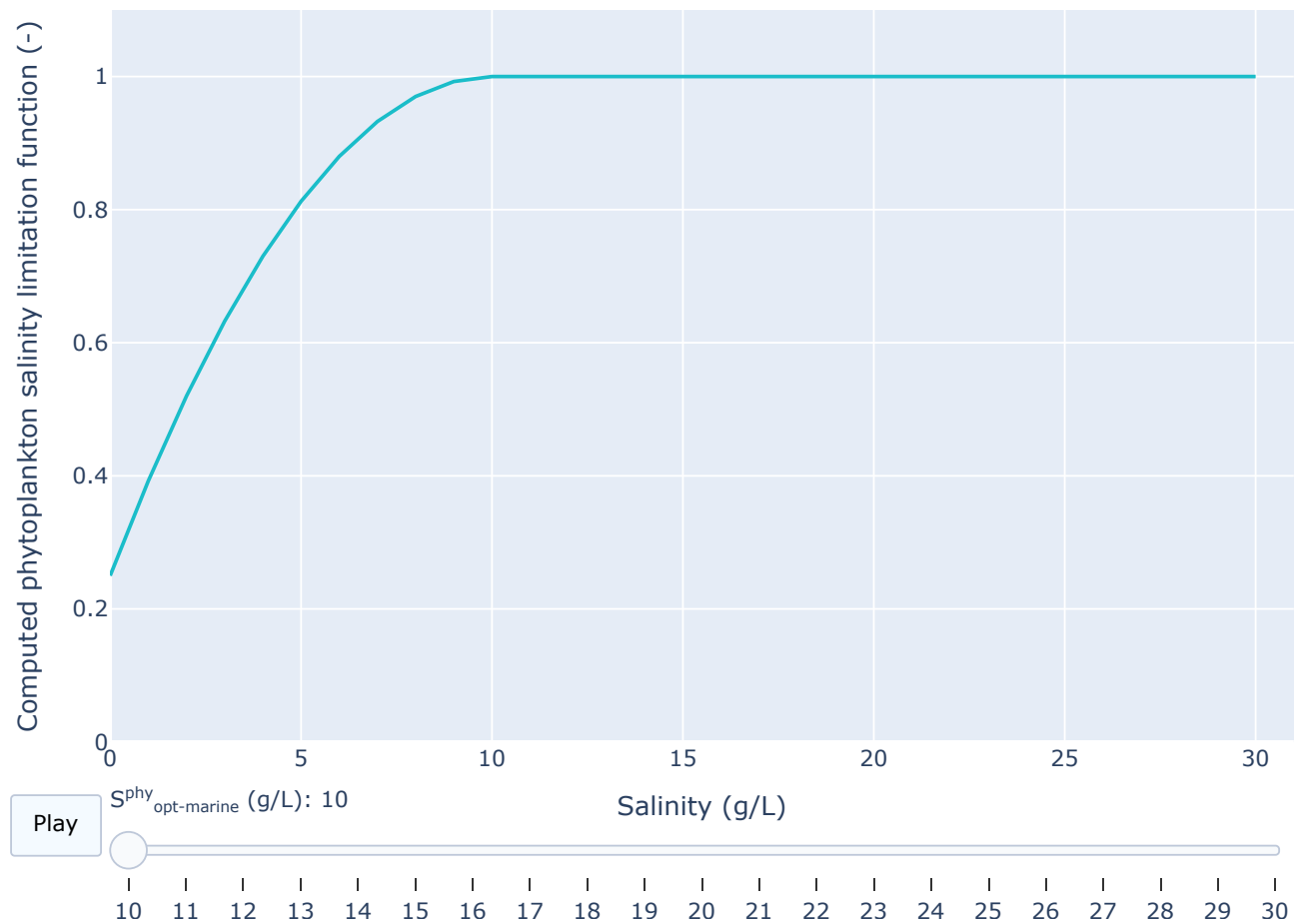


Figure I.15: Move the slider to see the effect of changing $S_{opt-marine}^{phy}$ on the computed salinity limitation function. $L_{zero-marine}^{phy} = 0.25$ and is fixed

I.7.3.2 Respiration

In order to apply this limitation function to respiration, $L_{zero-marine}^{phy}$ is set such that

$$1.0 < L_{zero-marine}^{phy} \quad (I.32)$$

In this case, and with decreasing salinity, the limitation function increases from 1.0 at $S_{opt-marine}^{phy}$ to a specified (or default) limitation function value at zero salinity.

For example, if a particular phytoplankton group was known to feel the effects of salinity on respiration below a salinity of 5 g/L, such that at a salinity of 0 g/L its respiration rate doubled, then the following would be set by the user:

- $S_{opt-marine}^{phy} = 5.0$ g/L
- $L_{zero-marine}^{phy} = 2.0$

Using these values initially but varying $S_{zero-marine}^{phy}$, the form of Equation I.30 is presented in Figure I.16.

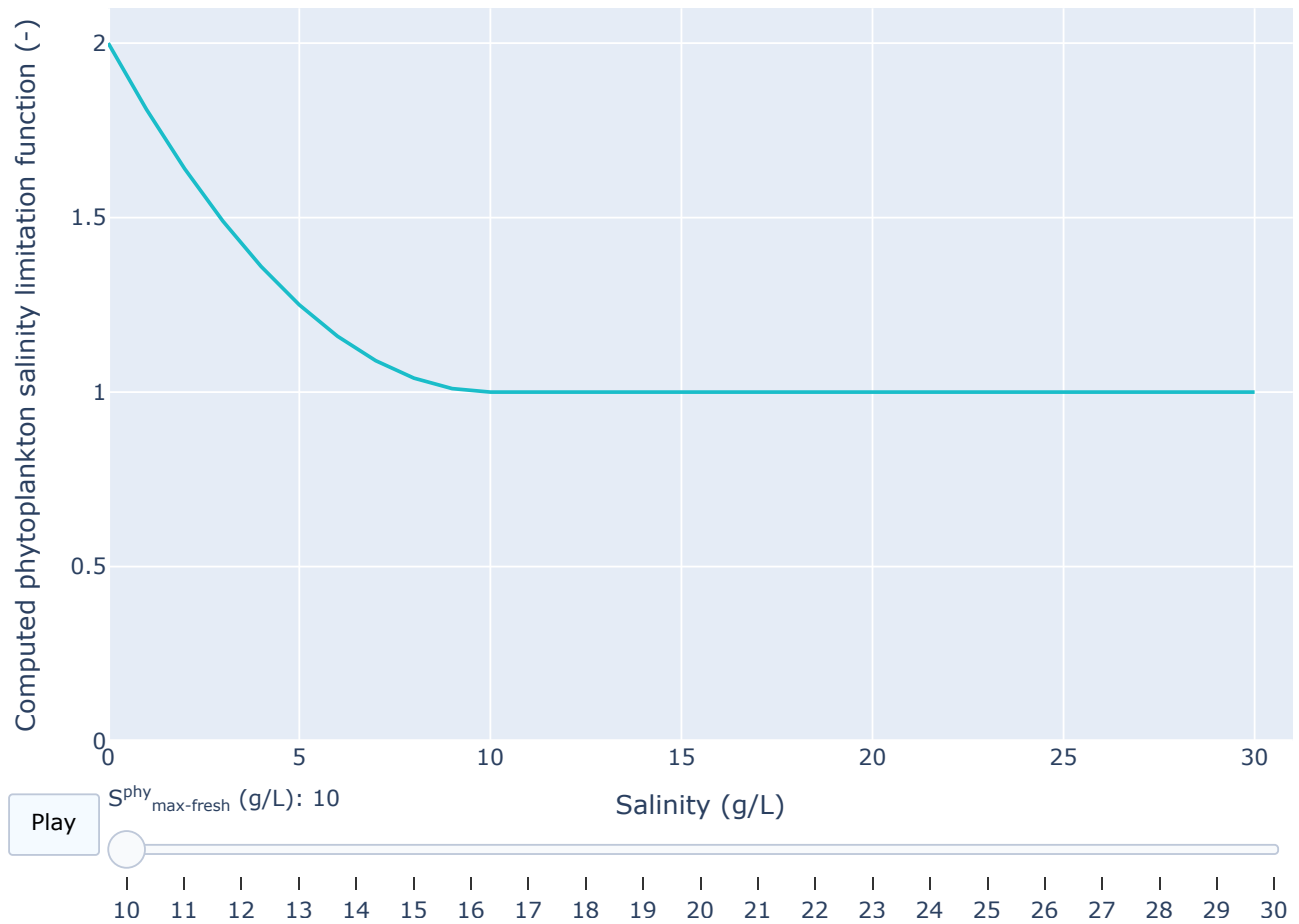


Figure I.16: Move the slider to see the effect of changing $S_{opt_marine}^{phy}$ on the computed salinity limitation function. $L_{zero-marine}^{phy} = 2.0$ and is fixed

1.7.4 Mixed

This model is typically used for phytoplankton groups that have a preference for mid range salinity waters. As such, the salinity limitation is set to 1.0 between specified (or default) optimal and maximum salinities. The general expression for the limitation function above and below this range is presented in Equation I.33, and this expression is applied to both primary productivity and respiration. Its specific applications to these two processes are described in the following subsections.

$$I_{sal-r}^{phy} = I_{sal-pp}^{phy} = \begin{cases} \left(\frac{(L_{zero-mix}^{phy} - 1.0) \times S^2}{(S_{opt-mix}^{phy})^2} \right) - \left(2.0 \times \frac{(L_{zero-mix}^{phy} - 1.0) \times S}{(S_{opt-mix}^{phy})} \right) + L_{zero-mix}^{phy} & S \leq S_{opt-mix}^{phy} \\ 1.0 & S_{opt-mix}^{phy} < S \leq S_{max-mix}^{phy} \\ \left(\frac{(L_{zero-mix}^{phy} - 1.0) \times (S_{max-mix}^{phy} + S_{opt-mix}^{phy} - S)^2}{(S_{opt-mix}^{phy})^2} \right) - \dots & \\ \dots \left(2.0 \times \frac{(L_{zero-mix}^{phy} - 1.0) \times (S_{max-mix}^{phy} + S_{opt-mix}^{phy} - S)}{(S_{opt-mix}^{phy})} \right) + L_{zero-mix}^{phy} & S_{max-mix}^{phy} < S \leq (S_{max-mix}^{phy} + S_{opt-mix}^{phy}) \\ L_{zero-mix}^{phy} & (S_{max-mix}^{phy} + S_{opt-mix}^{phy}) < S \end{cases} \quad (I.33)$$

$S_{opt-mix}^{phy}$ and $S_{max-mix}^{phy}$ are the optimal and maximum salinities, respectively, $L_{zero-mix}^{phy}$ is the value of the salinity limitation function at salinities of zero and greater than $(S_{opt-mix}^{phy} + S_{max-mix}^{phy})$ and S is ambient salinity.

1.7.4.1 Primary productivity

In order to apply this limitation function to primary productivity, $L_{zero-mix}^{phy}$ is set such that

$$0.0 \leq L_{zero-mix}^{phy} \leq 1.0 \quad (I.34)$$

In this case, the limitation function:

- Decreases at salinities below $S_{opt-mix}^{phy}$ to $L_{zero-mix}^{phy}$ at a salinity of zero, and
- Decreases at salinities above $S_{max-mix}^{phy}$ to $L_{zero-mix}^{phy}$ at a salinity equal to the sum of the specified optimal and maximum salinities

The simplest application of this limitation function is to set $L_{zero-mix}^{phy}$ to zero. This will ensure that no primary productivity occurs both at zero salinity and above a salinity of $S_{opt-mix}^{phy} + S_{max-mix}^{phy}$. For example, if a particular phytoplankton group was known to prefer salinities between 5 and 10 g/L, then the following would be set by the user:

- $S_{opt-mix}^{phy} = 5.0$ g/L
- $S_{max-mix}^{phy} = 10.0$ g/L
- $L_{zero-mix}^{phy} = 0.0$

Using these values initially but varying $S_{opt-mix}^{phy}$, the form of Equation I.33 is presented in Figure I.17. The absolute range between $S_{opt-mix}^{phy}$ and $S_{max-mix}^{phy}$ is held constant at 5.0 g/L for ease of comparison, so $S_{max-mix}^{phy}$ increases at the same rate as $S_{opt-mix}^{phy}$ when the slider moves.

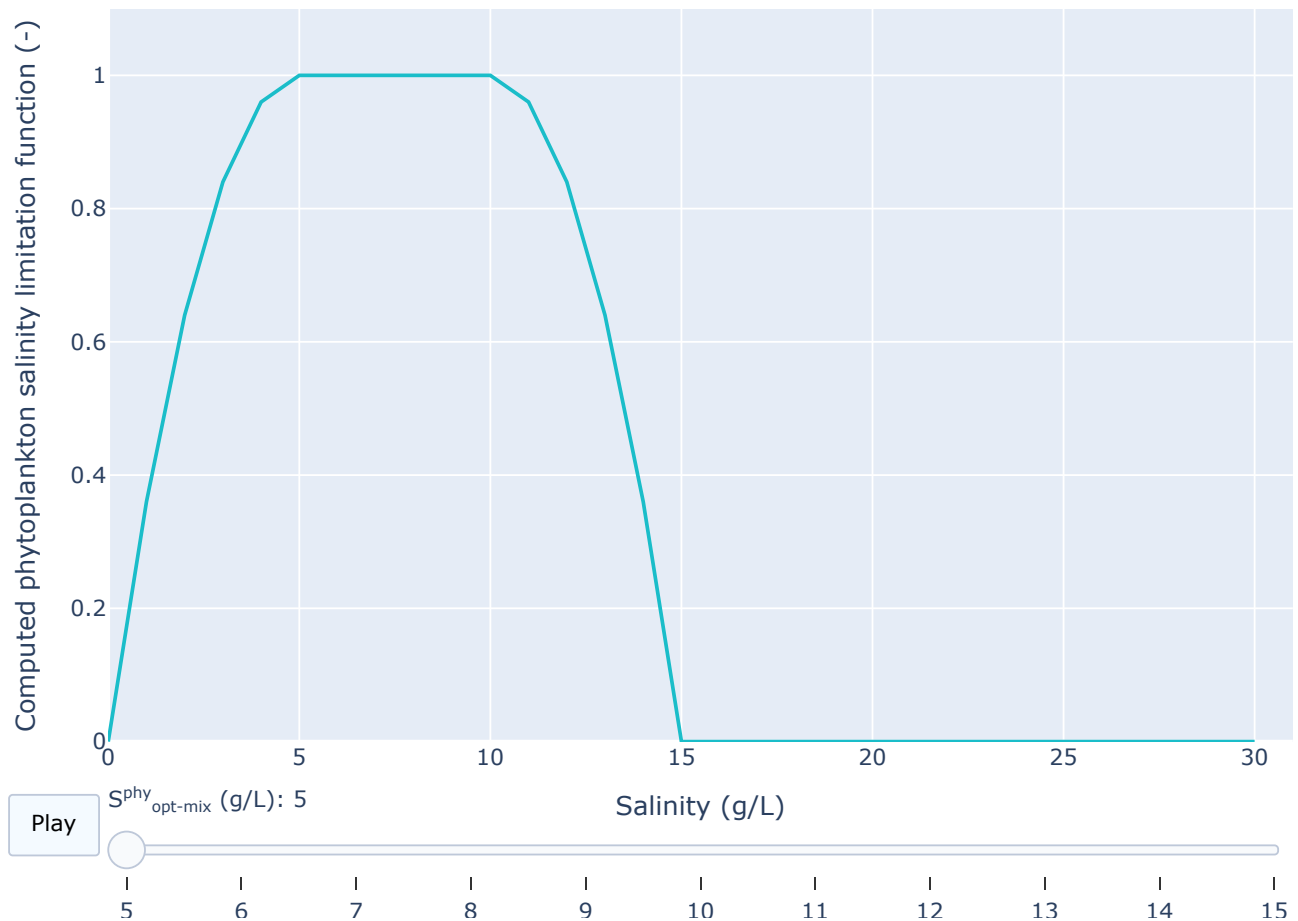


Figure I.17: Move the slider to see the effect of changing $S_{opt-mix}^{phy}$ on the computed salinity limitation function.
 $L_{zero-mix}^{phy} = 0.0$ and is fixed. $S_{max-mix}^{phy}$ is set to be $S_{opt-mix}^{phy} + 5.0$ g/L

Another example is the case where $L_{zero-mix}^{phy}$ is not zero. For example, if a particular phytoplankton group was known to prefer salinities between 5 and 10 g/L and have a 60% limitation on productivity at zero salinity, then the following would be set by the user:

- $S_{opt-mix}^{phy} = 5.0$ g/L
- $S_{max-mix}^{phy} = 10.0$ g/L
- $L_{zero-mix}^{phy} = 0.4$

Using these values initially but varying $S_{opt-mix}^{phy}$, the form of Equation I.33 is presented in Figure I.18. The absolute range between $S_{opt-mix}^{phy}$ and $S_{max-mix}^{phy}$ is again held constant at 5.0 g/L for ease of comparison, so $S_{max-mix}^{phy}$ increases at the same rate as $S_{opt-mix}^{phy}$ when the slider moves.

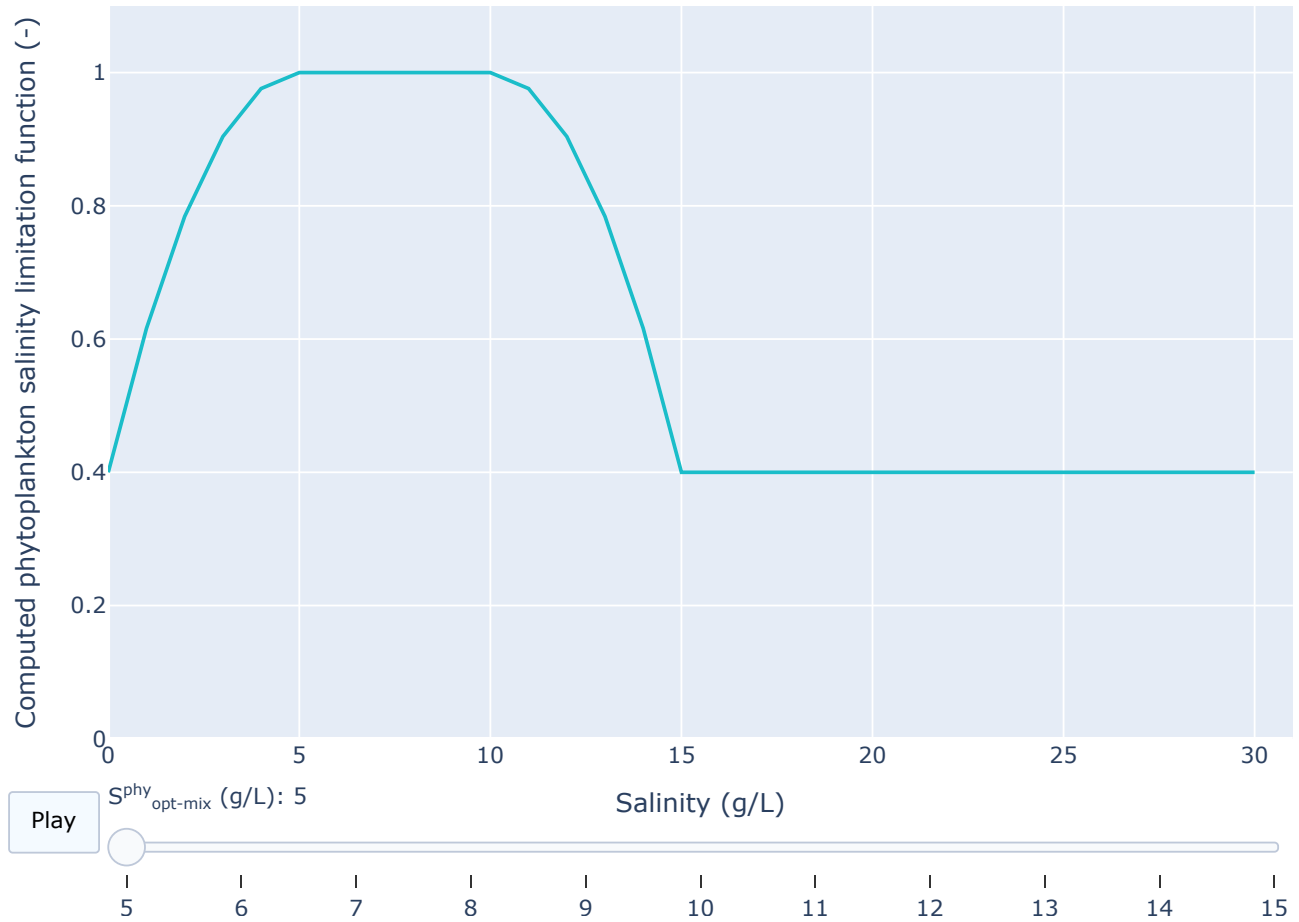


Figure I.18: Move the slider to see the effect of changing $S_{opt-mix}^{phy}$ on the computed salinity limitation function.

$L_{zero-mix}^{phy} = 0.4$ and is fixed. $S_{max-mix}^{phy}$ is set to be $S_{opt-mix}^{phy} + 5.0$ g/L

I.7.4.2 Respiration

In order to apply this limitation function to respiration, $L_{zero-mix}^{phy}$ is set such that

$$1.0 < L_{zero-mix}^{phy} \quad (I.35)$$

In this case, the limitation function:

- Increases at salinities below $S_{opt-mix}^{phy}$ to $L_{zero-mix}^{phy}$ at a salinity of zero, and
- Increases at salinities above $S_{max-mix}^{phy}$ to $L_{zero-mix}^{phy}$ at a salinity equal to the sum of the specified optimal and maximum salinities

For example, if a particular phytoplankton group was known to prefer salinities between 5 and 10 g/L but feel the effects of salinity outside this range such that at a salinity of zero its respiration rate doubled, then the following would be set by the user:

- $S_{opt-mix}^{phy} = 5.0$ g/L
- $S_{max-mix}^{phy} = 10.0$ g/L
- $L_{zero-mix}^{phy} = 2.0$

Using these values initially but varying $S_{opt-mix}^{phy}$, the form of Equation I.33 is presented in Figure I.19. The absolute range between $S_{opt-mix}^{phy}$ and $S_{max-mix}^{phy}$ is again held constant at 5.0 g/L for ease of comparison, so $S_{max-mix}^{phy}$ increases at the same rate as $S_{opt-mix}^{phy}$ when the slider moves.

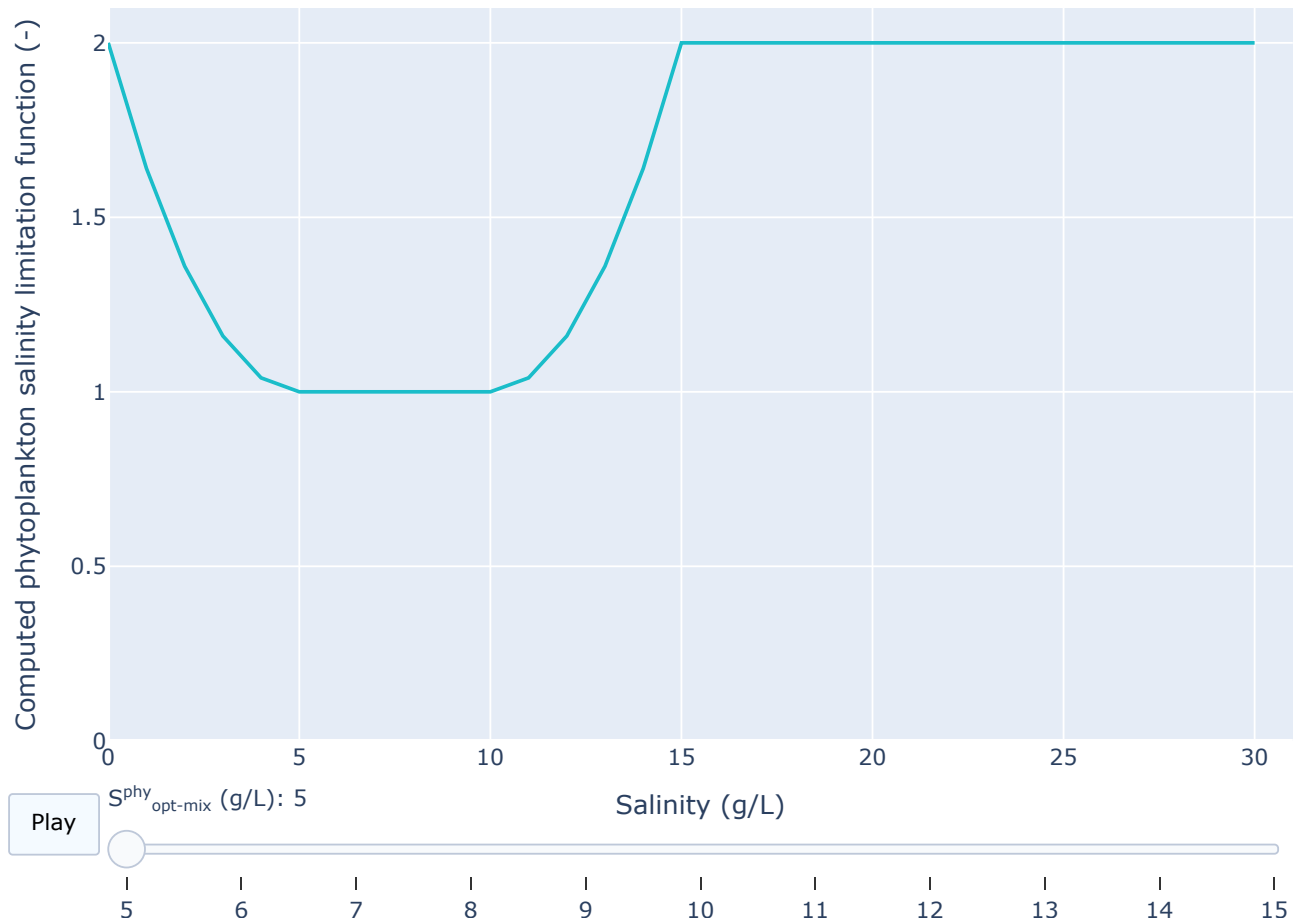


Figure I.19: Move the slider to see the effect of changing $S_{opt-mix}^{phy}$ on the computed salinity limitation function.

$L_{zero-mix}^{phy} = 2.0$ and is fixed. $S_{max-mix}^{phy}$ is set to be $S_{opt-mix}^{phy} + 5.0$ g/L

I.7.5 Estuarine

This model is typically used for phytoplankton groups that have a preference for brackish (typically estuarine) waters. As such, the salinity limitation is set to one at a specified (or default) optimal mid range salinity. The general expression for the limitation function above and below this salinity is presented in Equation I.36, and this expression is applied only to primary productivity.

$$I_{sal}^{phy} = \begin{cases} e^{P_{est}^{phy}(S - S_{opt-est}^{phy})} \times \left(\frac{(S_{max-est}^{phy} - S)}{(S_{max-est}^{phy} - S_{opt-est}^{phy})} \right)^{P_{est}^{phy}(S_{max-est}^{phy} - S_{opt-est}^{phy})} & S \leq S_{max-est}^{phy} \\ 0.0 & S_{max-est}^{phy} < S \end{cases} \quad (I.36)$$

$S_{opt-est}^{phy}$ and $S_{max-est}^{phy}$ are the optimal and maximum salinities, respectively, P_{est}^{phy} is the power coefficient and S is ambient salinity.

The intention of applying this limitation function is that it be applied to a relatively narrow band of mid range (estuarine or brackish) salinities. For example, if a particular phytoplankton group was known to produce optimally at a salinity of 15 g/L but had its growth completely suppressed less than 5 g/L and greater than 20 g/L, then the following would be set by the user:

- $S_{opt-est}^{phy} = 15.0$ g/L
- $S_{max-est}^{phy} = 20.0$ g/L
- $P_{est}^{phy} = 1.6$ (or greater)

Using these values but varying P_{est}^{phy} , the form of Equation I.36 is presented in Figure I.20. $S_{opt-est}^{phy}$ and $S_{max-est}^{phy}$ are held constant at 15.0 g/L and 20 g/L, respectively. The slider starts at a P_{est}^{phy} value of 0.2, and the key feature to note is that the salinity limitation function distribution tightens as P_{est}^{phy} increases.

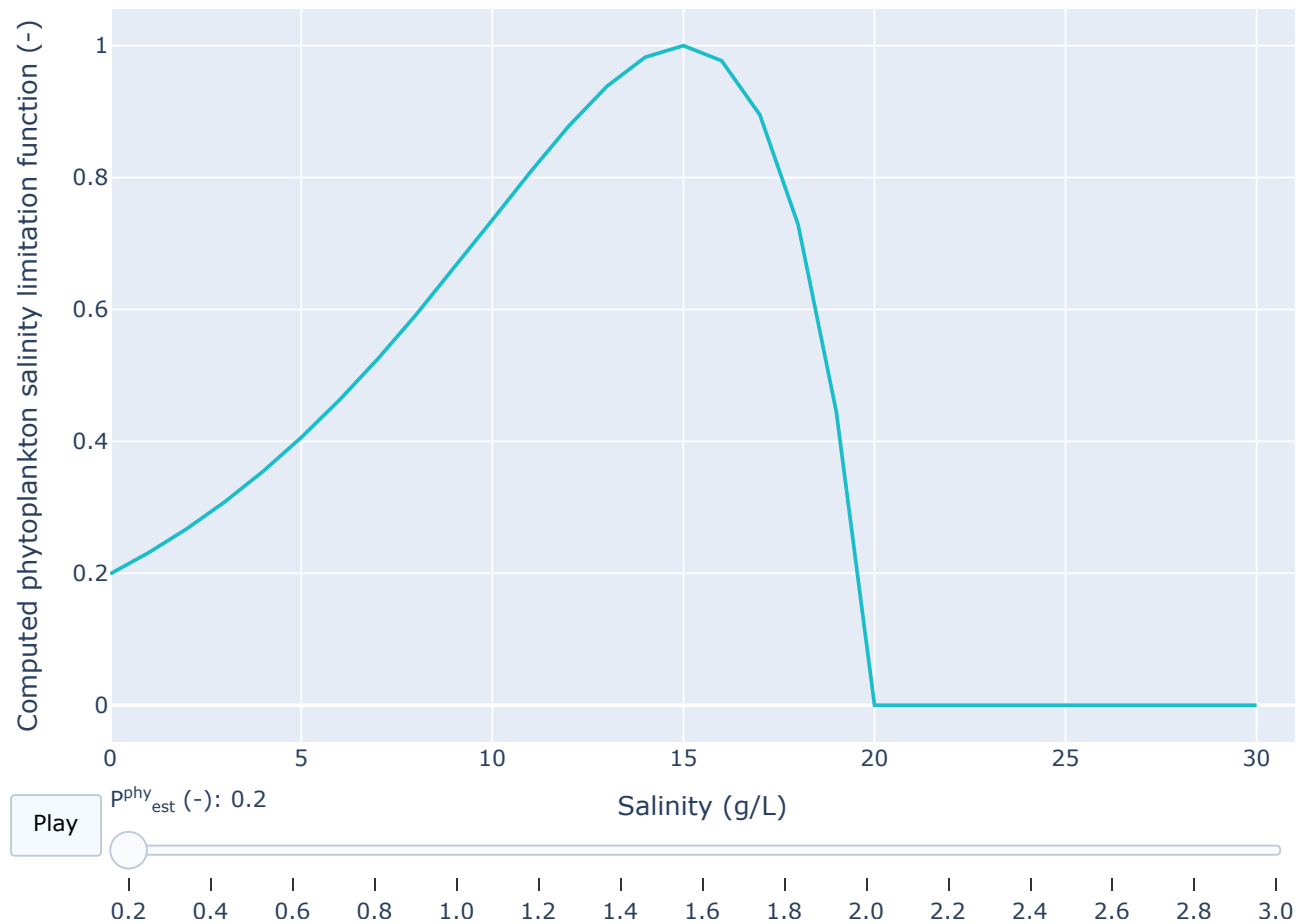


Figure I.20: Move the slider to see the effect of changing P_{est}^{phy} on the computed salinity limitation function.
 $S_{opt-est}^{phy}$ and $S_{max-est}^{phy}$ are set to be 15 and 20 g/L, respectively, and are fixed

J Processes: phyto uptake

Once the primary productivity $R_{prod(computed)}^{phy}$ rate has been computed for a phytoplankton group via Equation H.2 (and potentially Equation H.3 and Equation H.4 if nitrogen fixing and salinity limitation are activated, respectively), then that rate drives the mass uptake of inorganic carbon, nitrogen, phosphorus and silicate. This uptake includes the operation of a number of user specified (or default) parameters, and the respective calculations are described following. Uptakes are denoted as fluxes, F .

J.1 Carbon

Carbon has the simplest uptake calculation, as per Equation J.1.

$$F_{C-uptake}^{phy} = R_{prod(computed)}^{phy} \times [PHY] \quad (J.1)$$

$F_{C-uptake}^{phy}$ is the uptake of carbon, $R_{prod(computed)}^{phy}$ is the computed primary productivity rate and $[PHY]$ is a computational cell's phytoplankton concentration. This flux is summed over all simulated phytoplankton groups to compute the community carbon uptake, $F_{C-uptake(computed)}^{comm}$.

Carbon does not need to be explicitly simulated as a computed variable for this uptake to occur, but because carbon is used as the units of accounting for phytoplankton biomass, its uptake is computed by the WQ Module in order to report phytoplankton concentrations. These concentrations are either mmol C per m³ or µg chlorophyll *a* per litre (using a specified or default conversion), depending on the specified simulation units system. Carbon stores from which phytoplankton uptake can draw are assumed to be unlimited and unaccounted for when carbon is not explicitly included in a simulation as a computed variable.

J.2 Nitrogen

The WQ Module allows for phytoplankton to uptake nitrate and ammonium (i.e. inorganic nitrogen) to meet primary production nitrogen demands. The parallel uptake of organic nitrogen (i.e. simulation of mixotrophic phytoplankton) is not yet implemented within the WQ Module. Uptake is computed differently for the basic and advanced phytoplankton constituent models

J.2.1 Basic phytoplankton constituent model

If internal phytoplankton nutrients are not simulated dynamically, nitrogen uptake is calculated as per Equation J.2.

$$F_{N-uptake}^{phy} = R_{prod(computed)}^{phy} \times [PHY] \times X_{N-C-con}^{phy} \quad (J.2)$$

$F_{N-uptake}^{phy}$ is the uptake of water column inorganic nitrogen, $R_{prod(computed)}^{phy}$ is the computed primary productivity rate, $[PHY]$ is a computational cell's phytoplankton concentration and $X_{N-C-con}^{phy}$ is the specified (or default) constant ratio of internal nitrogen to carbon in the phytoplankton group being considered.

This quantity $F_{N-uptake}^{phy}$ is the total uptake of inorganic nitrogen. In order to disaggregate this uptake into that of ammonium and nitrate, the WQ Module applies Equation J.3, for ammonium concentrations greater than zero.

$$\left. \begin{aligned}
 f_{amm-uptake}^{phy} &= \frac{[NH_4] \times [NO_3]}{([NH_4] + K_{lim-N}^{phy}) \times ([NO_3] + K_{lim-N}^{phy})} + \frac{[NH_4] \times K_{lim-N}^{phy}}{([NH_4] + [NO_3]) \times ([NO_3] + K_{lim-N}^{phy})} \\
 F_{amm-uptake}^{phy} &= F_{N-uptake}^{phy} \times f_{amm-uptake}^{phy} \\
 F_{nit-uptake}^{phy} &= F_{N-uptake}^{phy} \times (1.0 - f_{amm-uptake}^{phy})
 \end{aligned} \right\} \quad (J.3)$$

For a phytoplankton group, $f_{amm-uptake}^{phy}$ is the fraction of nitrogen uptake that is ammonium, $[NH_4]$ and $[NO_3]$ are the ambient water column ammonium and nitrate concentrations, respectively, K_{lim-N}^{phy} is the half saturation nitrogen concentration for phytoplankton uptake and $F_{amm-uptake}^{phy}$ and $F_{nit-uptake}^{phy}$ are the uptake by phytoplankton of ammonium and nitrate, respectively. These fluxes (whether computed from Equation J.3 or Equation J.4) are summed over all simulated phytoplankton groups to compute the community ammonium and nitrate uptake, $F_{amm-uptake}^{comm}(\text{computed})$ and $F_{nit-uptake}^{comm}(\text{computed})$, respectively.

The form of $f_{amm-uptake}^{phy}$ in Equation J.3 with ammonium concentration is presented in Figure J.1. Use the “play” button or drag the slider to see how different half saturation concentrations K_{lim-N}^{phy} change the fraction of ammonium taken up by phytoplankton (ordinate), as a function of ambient ammonium concentration (abscissa). Nitrate concentration is set to a fixed 5 mg/L.

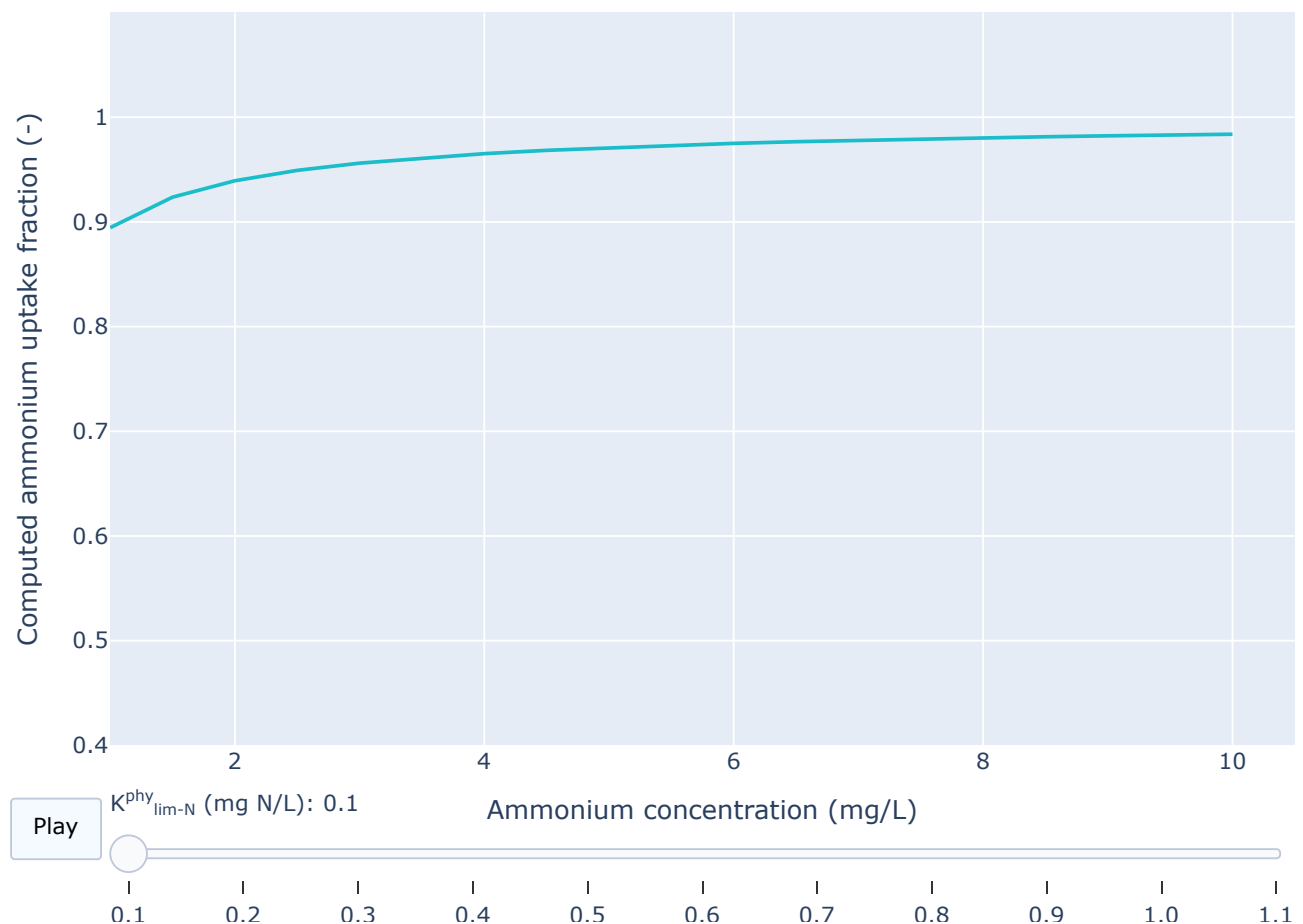


Figure J.1: Move the slider to see the effect of changing K_{lim-N}^{phy} on the fraction of ammonium taken up by phytoplankton. Nitrate concentration is set to 5 mg/L and is fixed

To complement Figure J.1, the form of $f_{amm-uptake}^{phy}$ in Equation J.3 with nitrate concentration is presented in Figure J.2, using the same ordinate axis limits. Use the “play” button or drag the slider to see how different half saturation

concentrations K_{lim-N}^{phy} change the fraction of ammonium taken up by phytoplankton (ordinate), as a function of ambient nitrate concentration (abscissa). Ammonium concentration is set to a fixed 2 mg/L.

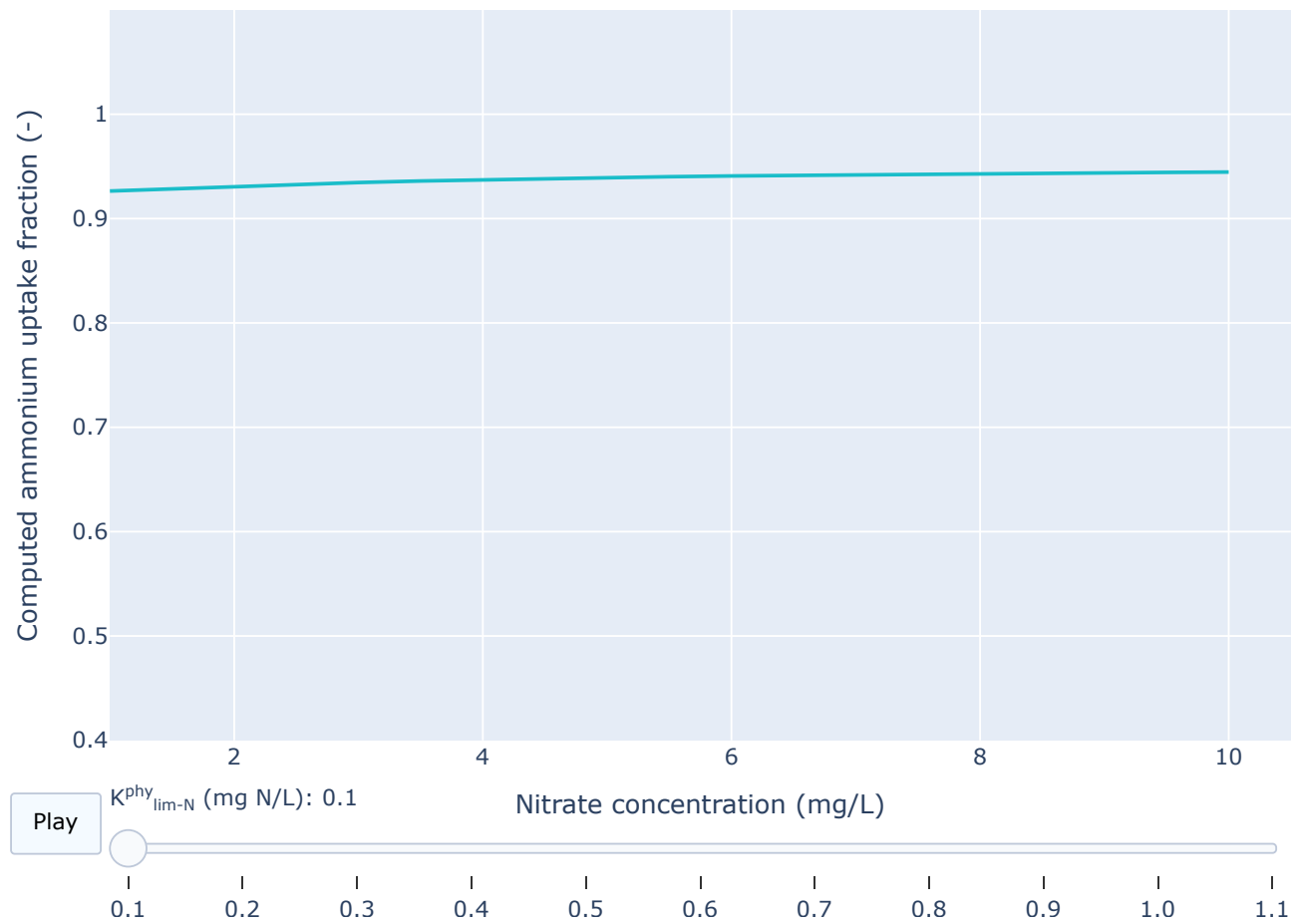


Figure J.2: Move the slider to see the effect of changing K_{lim-N}^{phy} on the fraction of ammonium taken up by phytoplankton. Ammonium concentration is set to 2 mg/L and is fixed

The parameter K_{lim-N}^{phy} is the same as that used for calculation of the nitrogen limitation function in the basic (and advanced if internal nitrogen stores are exhausted) phytoplankton constituent model, so its specification should be considered in terms of its influence on both uptake on limitation.

J.2.2 Advanced phytoplankton constituent model

If internal phytoplankton nutrients are simulated dynamically, nitrogen uptake is calculated as per Equation J.4.

$$F_{N-uptake}^{phy} = R_{N-uptake}^{phy} \times L_T^{phy} \times [PHY] \times \frac{(X_{N-C-max}^{phy} - \frac{[IN]}{[PHY]})}{(X_{N-C-max}^{phy} - X_{N-C-min}^{phy})} \times \frac{([N]_{avail} - [N]_{min})}{([N]_{avail} - [N]_{min}) + K_{lim-N}^{phy}} \quad (J.4)$$

$F_{N-uptake}^{phy}$ is the uptake of water column inorganic nitrogen, $R_{N-uptake}^{phy}$ is the specified (or default) rate of uptake of inorganic nitrogen, L_T^{phy} is the temperature limitation function, $[PHY]$ and $[IN]$ are a computational cell's phytoplankton and internal nitrogen concentrations respectively, $X_{N-C-min}^{phy}$ and $X_{N-C-max}^{phy}$ are the specified (or default) minimum and maximum ratios of internal nitrogen to carbon in the phytoplankton group being considered, respectively, $[N]_{avail}$ is the available (water column) nitrogen pool on which phytoplankton can draw for primary productivity, and is the sum of inorganic (ammonium and nitrate) nitrogen, $[N]_{min}^{phy}$ is the nitrogen concentration below which phytoplankton is no longer permitted to uptake nitrogen and K_{lim-N}^{phy} is the half saturation nitrogen concentration for phytoplankton uptake. These last three parameters (and the last term in Equation J.4) are the same as that applied to the basic phytoplankton

constituent model as per Equation J.2, via calculation of the limitation function applied to $R_{prod(computed)}^{phy}$ (as per Equation I.9).

Equation J.4 reveals the following:

- The uptake of water column nitrogen to internal phytoplankton stores is governed by the specified (or default) nitrogen uptake rate
- This rate is modified by
 - Temperature, using the specified (or default) temperature limitation model for uptake (Section I.2)
 - The current internal nitrogen concentrations, relative to the specified (or default) minima and maxima
 - Ambient water column inorganic nitrogen concentrations, and
 - The half saturation nitrogen concentration for uptake, which is the same parameter as used in the basic phytoplankton constituent model

If for example the internal nitrogen concentration $[IN]$ at a particular timestep and computational cell is equal to $X_{N-C-max}^{phy} \times [PHY]$, then Equation J.4 has that internal nitrogen stores are full and that uptake is therefore zero. Conversely, if $[IN]$ at a particular timestep and computational cell is equal to $X_{N-C-min}^{phy} \times [PHY]$, then internal nitrogen stores are at their lowest and therefore (in themselves) do not limit uptake of water column nitrogen. Finally, if the available water column nitrogen $[N]_{avail}$ is equal to the specified (or default) minimum allowable nitrogen concentration for uptake $[N]_{min}^{phy}$, then uptake to internal nutrient stores is zero.

If uptake from the water column to internal stores occurs, then the split between ammonium and nitrate uptake is computed as per Equation J.3.

The parameter K_{lim-N}^{phy} is the same as that used for calculation of the nitrogen limitation function in the advanced phytoplankton constituent model if internal nitrogen stores are exhausted, so its specification should be considered in terms of its influence on both uptake on limitation.

J.2.3 Nitrogen fixing

If nitrogen fixing by phytoplankton is simulated, then a modification to the above computed nitrogen uptakes (for both the basic and advanced phytoplankton constituent models) is applied. The flux of atmospheric nitrogen is computed as per Equation J.5.

$$F_{N-fix}^{phy} = R_{N-fix}^{phy} \times (1.0 - L_{nit}^{phy}) \times [PHY] \quad (J.5)$$

F_{N-fix}^{phy} is the fixing of atmospheric nitrogen, R_{N-fix}^{phy} is the specified (or default) rate of nitrogen fixing, L_{nit}^{phy} is the nitrogen limitation function computed via either Equation I.9 or Equation I.11 for the basic and advanced phytoplankton constituent models, respectively, before L_{nit}^{phy} is set to one. Once computed, $F_{N-uptake}^{phy}$ is modified as follows:

- If $|F_{N-fix}^{phy}| \geq |F_{N-uptake}^{phy}|$ then all uptake is assigned to F_{N-fix}^{phy} , and $F_{N-uptake}^{phy}$ is set to zero.
- If $|F_{N-fix}^{phy}| \leq |F_{N-uptake}^{phy}|$ then nitrogen water column uptake is reduced as per Equation J.6.

$$F_{N-uptake(computed)}^{phy} = F_{N-uptake}^{phy} \times \frac{(|F_{N-uptake}^{phy}| - F_{N-fix}^{phy})}{|F_{N-uptake}^{phy}|} \quad (J.6)$$

Equation J.6 is a simple linearisation that maps $F_{N-uptake(computed)}^{phy}$ to a value between 0.0 (where $F_{N-fix}^{phy} = F_{N-uptake}^{phy}$) and $F_{N-uptake(computed)}^{phy}$ (where F_{N-fix}^{phy} is zero).

J.3 Phosphorus

The WQ Module allows for phytoplankton to uptake filterable reactive phosphorus (i.e. inorganic phosphorus, FRP) to meet primary production phosphorus demands. The parallel uptake of organic phosphorus (i.e. simulation of mixotrophic phytoplankton) is not yet implemented within the WQ Module. Uptake is computed differently for the basic and advanced phytoplankton constituent models

J.3.1 Basic phytoplankton constituent model

If internal phytoplankton nutrients are not simulated dynamically, phosphorus uptake is calculated as per Equation J.7.

$$F_{P-uptake}^{phy} = R_{prod(computed)}^{phy} \times [PHY] \times X_{P-C-con}^{phy} \quad (J.7)$$

$F_{P-uptake}^{phy}$ is the uptake of inorganic phosphorus, $R_{prod(computed)}^{phy}$ is the computed primary productivity rate, $[PHY]$ is a computational cell's phytoplankton concentration and $X_{P-C-con}^{phy}$ is the specified (or default) constant ratio of internal phosphorus to carbon in the phytoplankton group being considered. This flux (whether computed from Equation J.7 or Equation J.8) is summed over all simulated phytoplankton groups to compute the community FRP uptake, $F_{P-uptake(community)}^{comm}$.

J.3.2 Advanced phytoplankton constituent model

If internal phytoplankton nutrients are simulated dynamically, phosphorus uptake is calculated as per Equation J.8.

$$F_{P-uptake}^{phy} = R_{P-uptake}^{phy} \times L_T^{phy} \times [PHY] \times \frac{(X_{P-C-max}^{phy} - \frac{[IP]}{[PHY]})}{(X_{P-C-max}^{phy} - X_{P-C-min}^{phy})} \times \frac{([P]_{avail} - [P]_{min}^{phy})}{([P]_{avail} - [P]_{min}^{phy}) + K_{lim-P}^{phy}} \quad (J.8)$$

$F_{P-uptake}^{phy}$ is the uptake of water column FRP, $R_{P-uptake}^{phy}$ is the specified (or default) rate of uptake of FRP, L_T^{phy} is the temperature limitation function, $[PHY]$ and $[IP]$ are a computational cell's phytoplankton and internal phosphorus concentrations respectively, $X_{P-C-min}^{phy}$ and $X_{P-C-max}^{phy}$ are the specified (or default) minimum and maximum ratios of internal phosphorus to carbon in the phytoplankton group being considered, respectively, $[P]_{avail}$ is the available (i.e. ambient water column) FRP pool on which phytoplankton can draw for primary productivity, $[P]_{min}^{phy}$ is the FRP concentration below which phytoplankton is no longer permitted to uptake phosphorus and K_{lim-P}^{phy} is the half saturation FRP concentration for phytoplankton uptake. These last three parameters (and the last term in Equation J.8) are the same as that applied to the basic phytoplankton constituent model as per Equation J.7, via calculation of the limitation function applied to $R_{prod(computed)}^{phy}$ (as per Equation I.13).

Equation J.8 reveals the following:

- The uptake of water column FRP to internal phytoplankton stores is governed by the specified (or default) phosphorus uptake rate
- This rate is modified by
 - Temperature, using the specified (or default) temperature limitation model for uptake (Section I.2)
 - The current internal phosphorus concentrations, relative to the specified (or default) minima and maxima
 - Ambient water column FRP concentrations, and
 - The half saturation phosphorus concentration for uptake, which is the same parameter as used in the basic phytoplankton constituent model

If for example the internal phosphorus concentration $[IP]$ at a particular timestep and computational cell is equal to $X_{P-C-max}^{phy} \times [PHY]$, then Equation J.8 has that internal phosphorus stores are full and that uptake is therefore zero. Conversely, if $[IP]$ at a particular timestep and computational cell is equal to $X_{P-C-min}^{phy} \times [PHY]$, then internal phosphorus stores are at their lowest and therefore (in themselves) do not limit uptake of water column FRP. Finally, if the available water column FRP $[P]_{avail}$ is equal to the specified (or default) minimum allowable FRP concentration for uptake $[P]_{min}^{phy}$, then uptake to internal nutrient stores is zero.

The parameter K_{lim-P}^{phy} is the same as that used for calculation of the phosphorus limitation function in the advanced phytoplankton constituent model if internal phosphorus stores are exhausted, so its specification should be considered in terms of its influence on both uptake on limitation.

J.4 Silicate

The WQ Module allows for phytoplankton to uptake silicate to meet primary production demands, for phytoplankton groups that require silicate. Silicate uptake is calculated as per Equation J.9.

$$F_{Si-uptake}^{phy} = R_{prod(computed)}^{phy} \times [PHY] \times X_{Si-C-con}^{phy} \quad (J.9)$$

$F_{Si-uptake}^{phy}$ is the uptake of silicate, $R_{prod(computed)}^{phy}$ is the computed primary productivity rate, $[PHY]$ is a computational cell's phytoplankton concentration and $X_{Si-C-con}^{phy}$ is the specified (or default) constant ratio of internal silicate to carbon in the phytoplankton group being considered.



K Processes: phyto losses

Once the respiration $R_{resp(computed)}^{phy}$ and exudation $R_{exud(computed)}^{phy}$ rates have been computed for a phytoplankton group via Equation H.6 and Equation H.12 respectively (and potentially Equation H.7 if salinity limitation is activated), then those rates drive the mass losses of carbon, nitrogen, phosphorus and silicate. These losses are computed using a number of user specified (or default) parameters, and for each relevant computed variable, comprise the following:

- Excretion loss: Computed from a combination of respiration and exudation rates ($R_{resp(computed)}^{phy}$ and $R_{exud(computed)}^{phy}$, respectively), and
- Mortality loss: Computed from the respiration rate $R_{resp(computed)}^{phy}$

The specifics of the calculation of each relevant computed variable's excretion and mortality are described following. Losses are denoted as fluxes, F .

K.1 Carbon

Equation K.1 describes the calculation of excretion losses.

$$F_{C-excr}^{phy} = \left(\left((1 - f_{true-resp}^{phy}) \times f_{excr-loss}^{phy} \times R_{resp(computed)}^{phy} \right) + R_{exud(computed)}^{phy} \right) \times [PHY] \quad (K.1)$$

F_{C-excr}^{phy} is the excretive loss of carbon and $f_{true-resp}^{phy}$ is the fraction of respiration that corresponds to the generation of energy via consumption of stored chlorophyll a (i.e. the fraction that does not result in excretive or mortality losses). In Equation K.1, $(1 - f_{true-resp}^{phy})$ is therefore the respiration that is associated with the combined excretive and mortality losses, rather than energy production. $f_{excr-loss}^{phy}$ is the fraction of this combined loss that is excretive only, $R_{resp(computed)}^{phy}$ and $R_{exud(computed)}^{phy}$ are the computed respiration and exudation rates, respectively and $[PHY]$ is a computational cell's phytoplankton concentration.

Equation K.2 describes the calculation of mortality losses of carbon.

$$F_{C-mort}^{phy} = \left((1 - f_{true-resp}^{phy}) \times (1 - f_{excr-loss}^{phy}) \times R_{resp(computed)}^{phy} \right) \times [PHY] \quad (K.2)$$

F_{C-mort}^{phy} is the mortality loss of carbon and the other terms in Equation K.2 as the same as Equation K.1, noting the inclusion of $(1 - f_{excr-loss}^{phy})$ in Equation K.2 to isolate the fraction of the combined excretive and mortality loss that is mortality only.

As with primary productivity, carbon does not need to be explicitly simulated as a computed variable for these losses to occur, but because carbon is used as the units of accounting for phytoplankton biomass, its losses are computed by the WQ Module in order to report phytoplankton concentrations. Carbon stores to which the phytoplankton losses in Equation K.1 and Equation K.2 deliver are assumed to be unlimited when carbon is not explicitly included in a simulation as a computed variable.

The form of the entire multiplicative factors immediately preceding $[PHY]$ in Equation K.1 and Equation K.2 are presented in Figure K.1, as a function of $f_{excr-loss}^{phy}$. Use the play button or drag the slider to see how different values of $f_{true-resp}^{phy}$ change these multiplicative factors (ordinate), which are shown as functions of $f_{excr-loss}^{phy}$ (abscissa). $R_{resp(computed)}^{phy}$ and $R_{exud(computed)}^{phy}$ are set to fixed values of 0.1 and 0.05 /day, respectively.

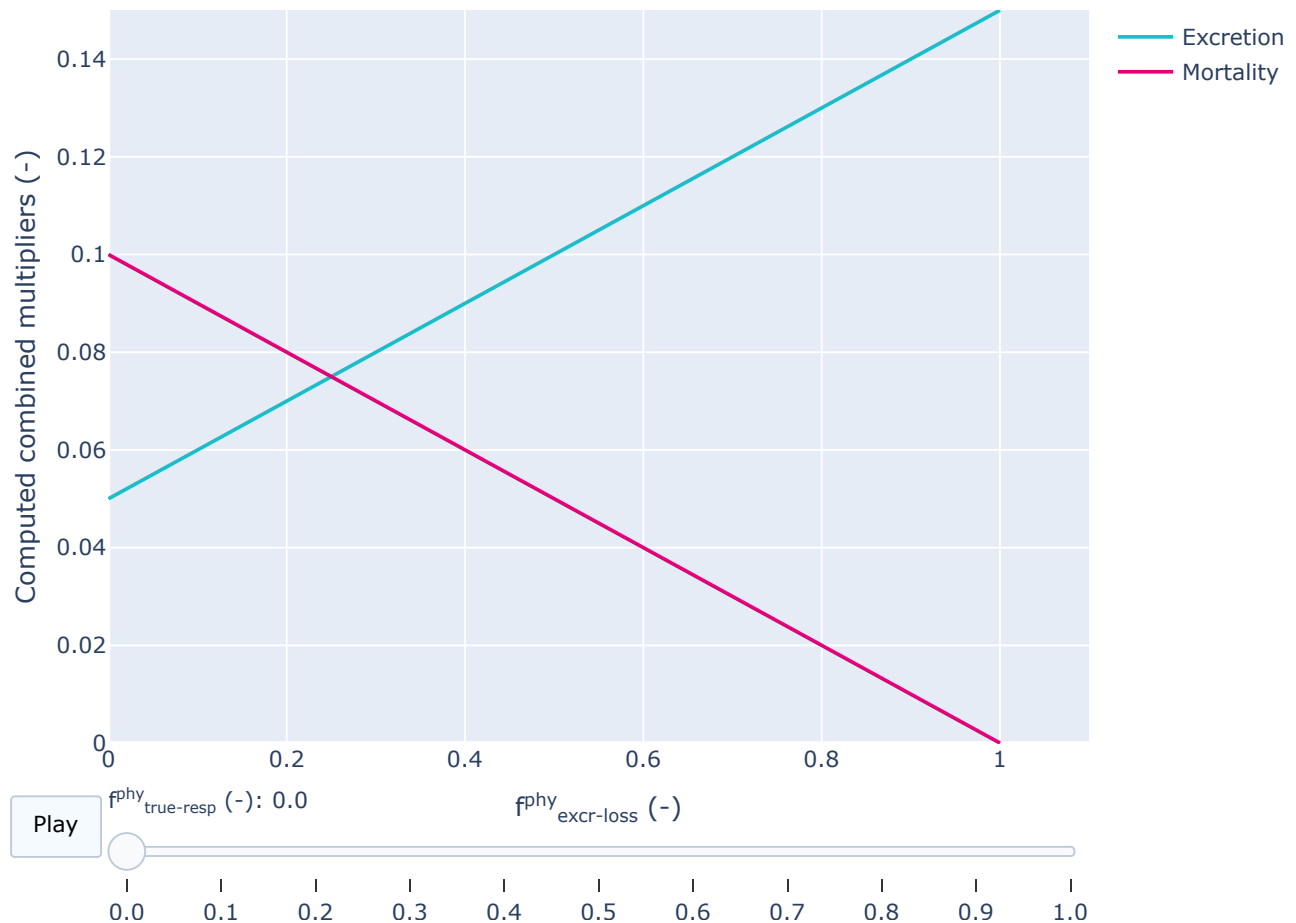


Figure K.1: Move the slider to see the effect of changing $f_{true-resp}^{phy}$ on the form of the multiplicative factors preceding $[PHY]$ in the above loss equations. $R_{resp<computed>}^{phy}$ and $R_{exud<computed>}^{phy}$ are set to fixed values of 0.1 and 0.05 /day, respectively

To complement Figure K.1, the form of the entire multiplicative factors immediately preceding $[PHY]$ in Equation K.1 and Equation K.2 are again presented in Figure K.2, but as a function of $f_{true-resp}^{phy}$. Use the play button or drag the slider to see how different values of $f_{excr-loss}^{phy}$ change these multiplicative factors (ordinate), which are shown as functions of $f_{true-resp}^{phy}$ (abscissa). $R_{resp<computed>}^{phy}$ and $R_{exud<computed>}^{phy}$ are again set to the same fixed values of 0.1 and 0.05 /day, respectively.

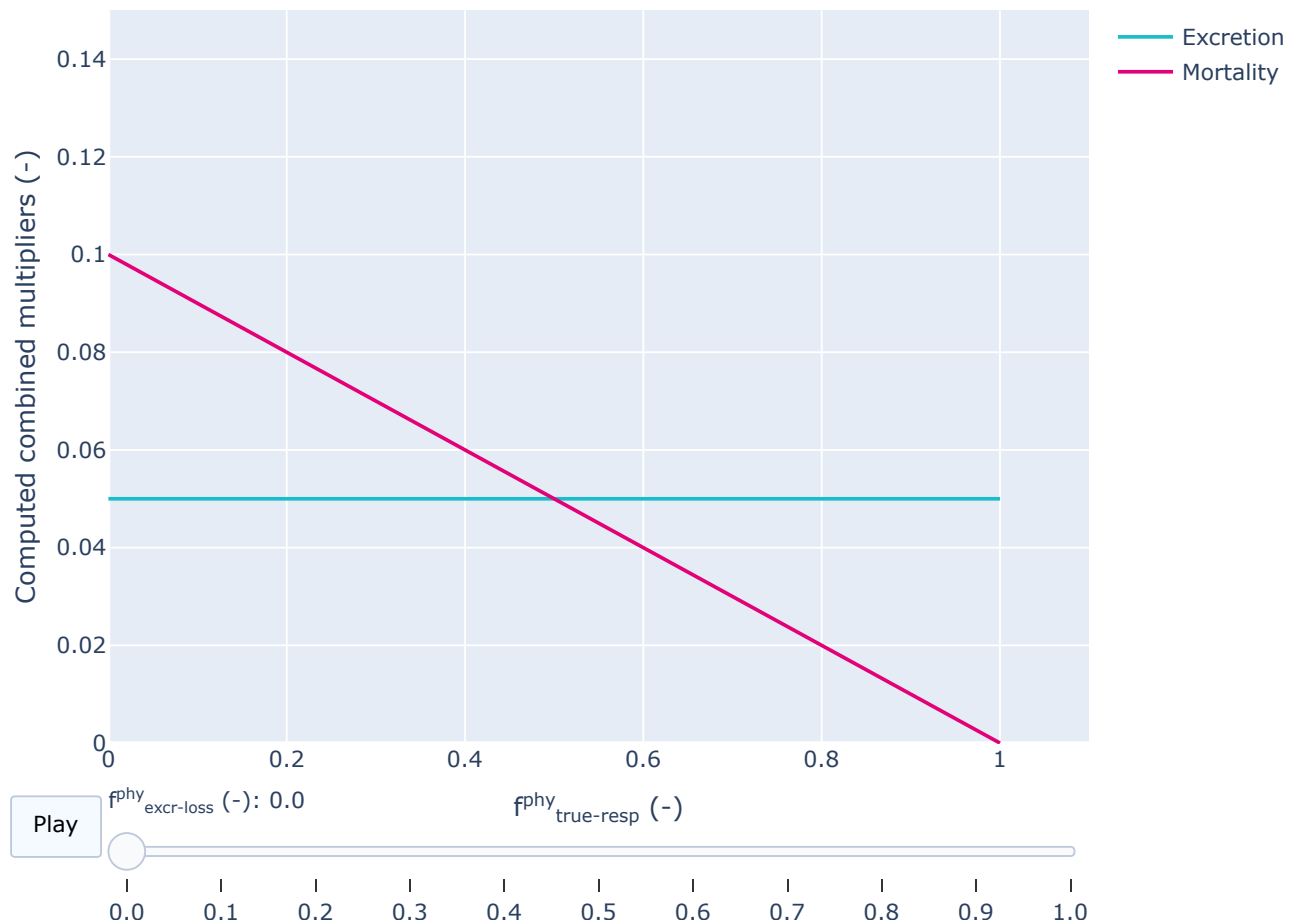


Figure K.2: Move the slider to see the effect of changing $f_{\text{phy}}^{\text{excr-loss}}$ on the form of the multiplicative factors preceding $[PHY]$ in the above loss equations. $R_{\text{resp}(\text{computed})}^{\text{phy}}$ and $R_{\text{exud}(\text{computed})}^{\text{phy}}$ are set to fixed values of 0.1 and 0.05 /day, respectively

Some key features of the Figure K.1 and Figure K.2 are as follows:

- If $f_{\text{true-resp}}^{\text{phy}}$ is set to 1.0, then carbonaceous excretion losses are due solely to exudation, and mortality losses are zero. This is consistent with interpreting $f_{\text{true-resp}}^{\text{phy}}$ as the fraction of respiration that is associated only with the re-release of energy through metabolism of carbon biomass generated and stored during antecedent phytoplanktonic photosynthesis
- Conversely, if $f_{\text{true-resp}}^{\text{phy}}$ is set to 0.0, then (potentially unrealistically) respiration does not re-release any energy, but rather, sees the entire respiration rate expended on excretion of carbon biomass (subject to the value of $f_{\text{excr-loss}}^{\text{phy}}$)
- If $f_{\text{excr-loss}}^{\text{phy}}$ is set to 1.0, then mortality losses are zero. This is consistent with interpreting this parameter as the proportion of combined excretive and mortality losses that are excretive. The converse applies for a $f_{\text{excr-loss}}^{\text{phy}}$ of 0.0

Intermediate behaviours to the above limits can be inferred through interacting with Figure K.1 and Figure K.2.

K.2 Nitrogen

Equation K.3 describes the calculation of excretion losses.

$$F_{N-\text{excr}}^{\text{phy}} = \left((f_{\text{excr-loss}}^{\text{phy}} \times R_{\text{resp}(\text{computed})}^{\text{phy}}) + R_{\text{exud}(\text{computed})}^{\text{phy}} \right) \times X_{N-C}^{\text{phy}} \times [PHY] \quad (\text{K.3})$$

$F_{N-\text{excr}}^{\text{phy}}$ is the excretive loss of nitrogen, $f_{\text{excr-loss}}^{\text{phy}}$ is the fraction of combined excretive and mortality losses that is excretive only, $R_{\text{resp}(\text{computed})}^{\text{phy}}$ and $R_{\text{exud}(\text{computed})}^{\text{phy}}$ are the computed respiration and exudation rates, respectively, and

$[PHY]$ is a computational cell's phytoplankton concentration. If the basic phytoplankton constituent model is used, then X_{N-C}^{phy} is the specified (or default) constant ratio of internal nitrogen to carbon. If the advanced phytoplankton constituent model is used, then X_{N-C}^{phy} is the dynamically computed ratio of internal nitrogen to carbon concentrations, where this ratio varies only between the specified (or default) minimum and maximum ratios $X_{N-C-min}^{phy}$ and $X_{N-C-max}^{phy}$, respectively.

Equation K.4 describes the calculation of mortality losses.

$$F_{N-mort}^{phy} = \left((1 - f_{excr-loss}^{phy}) \times R_{resp(computed)}^{phy} \right) \times X_{N-C}^{phy} \times [PHY] \quad (K.4)$$

F_{N-mort}^{phy} is the mortality loss of nitrogen and the other terms in Equation K.4 as the same as Equation K.3, noting the inclusion of $(1 - f_{excr-loss}^{phy})$ in Equation K.4 to isolate the fraction of the combined excretive and mortality loss that is mortality only.

The key feature of Equation K.3 and Equation K.4 is that if $f_{excr-loss}^{phy}$ is set to 1.0, then mortality losses are zero. This is consistent with interpreting this parameter as the proportion of combined excretive and mortality losses that are excretive. The converse applies for a $f_{excr-loss}^{phy}$ of 0.0.

K.3 Phosphorus

Equation K.5 describes the calculation of excretion losses.

$$F_{P-excr}^{phy} = \left((f_{excr-loss}^{phy} \times R_{resp(computed)}^{phy}) + R_{exud(computed)}^{phy} \right) \times X_{P-C}^{phy} \times [PHY] \quad (K.5)$$

F_{P-excr}^{phy} is the excretive loss of phosphorus, $f_{excr-loss}^{phy}$ is the fraction of combined excretive and mortality losses that is excretive only, $R_{resp(computed)}^{phy}$ and $R_{exud(computed)}^{phy}$ are the computed respiration and exudation rates, respectively, and $[PHY]$ is a computational cell's phytoplankton concentration. If the basic phytoplankton constituent model is used, then X_{P-C}^{phy} is the specified (or default) constant ratio of internal phosphorus to carbon. If the advanced phytoplankton constituent model is used, then X_{P-C}^{phy} is the dynamically computed ratio of internal phosphorus to carbon concentrations, where this ratio varies only between the specified (or default) minimum and maximum ratios $X_{P-C-min}^{phy}$ and $X_{P-C-max}^{phy}$, respectively.

Equation K.6 describes the calculation of mortality losses.

$$F_{P-mort}^{phy} = \left((1.0 - f_{excr-loss}^{phy}) \times R_{resp(computed)}^{phy} \right) \times X_{P-C}^{phy} \times [PHY] \quad (K.6)$$

F_{P-mort}^{phy} is the mortality loss of phosphorus and the other terms in Equation K.6 as the same as Equation K.5, noting the inclusion of $(1 - f_{excr-loss}^{phy})$ in Equation K.6 to isolate the fraction of the combined excretive and mortality loss that is mortality only.

As for nitrogen losses, the key feature of Equation K.5 and Equation K.6 is that if $f_{excr-loss}^{phy}$ is set to 1.0, then mortality losses are zero. This is consistent with interpreting this parameter as the proportion of combined excretive and mortality losses that are excretive. The converse applies for a $f_{excr-loss}^{phy}$ of 0.0.

K.4 Silicate

Equation K.7 describes the calculation of excretion losses, if silicate is included in phytoplanktonic calculations.

$$F_{Si-excr}^{phy} = \left((f_{excr-loss}^{phy} \times R_{resp(computed)}^{phy}) + R_{exud(computed)}^{phy} \right) \times X_{Si-C}^{phy} \times [PHY] \quad (K.7)$$

$F_{Si-excr}^{phy}$ is the excretive loss of silicate, $f_{excr-loss}^{phy}$ is the fraction of combined excretive and mortality losses that is excretive only, $R_{resp(computed)}^{phy}$ and $R_{exud(computed)}^{phy}$ are the computed respiration and exudation rates, respectively,

X_{Si-C}^{phy} is the specified (or default) constant ratio of internal silicate to carbon in the phytoplankton group being considered and $[PHY]$ is a computational cell's phytoplankton concentration.

Equation K.8 describes the calculation of mortality losses.

$$F_{Si-mort}^{phy} = \left((1.0 - f_{excr-loss}^{phy}) \times R_{resp(computed)}^{phy} \right) \times X_{Si-C}^{phy} \times [PHY] \quad (K.8)$$

Some key features of the Equation K.7 and Equation K.8 are as follows:

- As for nitrogen and phosphorus losses, the key feature of Equation K.7 and Equation K.8 is that if $f_{excr-loss}^{phy}$ is set to 1.0, then mortality losses are zero. This is consistent with interpreting this parameter as the proportion of combined excretive and mortality losses that are excretive. The converse applies for a $f_{excr-loss}^{phy}$ of 0.0
- Despite not simulating particulate silicate, Equation K.7 and Equation K.8 nonetheless ensure that the mass of silicate delivered to the dissolved pool (that is simulated by the WQ Module) is consistent with that of carbon, nitrogen and phosphorus.

L Processes: phyto other

L.1 Self shading

Photosynthetically available radiation is provided to the WQ Module from TUFLOW for each computational cell at each water quality timestep. It is this two- or three-dimensional field that the WQ Module uses to compute phytoplanktonic responses to light. The WQ Module allows, however, for modification of this TUFLOW field to incorporate the effect of light attenuation due to the presence of phytoplankton. This additional light extinction is computed dynamically at each water quality timestep, based on instantaneous phytoplanktonic concentrations in individual computational cells, as per Equation L.1.

$$Ke_{(computed)}^{phy} = Ke^{phy} \times [PHY] \quad (L.1)$$

For each phytoplankton group, Ke^{phy} is the user specified (or default) self shading coefficient and $[PHY]$ is the instantaneous phytoplankton concentration in each cell. For each cell and at each timestep, this quantity $Ke_{(computed)}^{phy}$ is computed for each phytoplankton group. Results are then summed within each cell and returned to TUFLOW as a two- or three-dimensional field which TUFLOW then includes these in subsequent light distribution calculations.

L.2 Cell density

The principle of the WQ Module density calculations is that cell density is set to increase during daylight primary production (when carbohydrates are created via photosynthesis) and decrease during darkness respiration (when carbohydrates are consumed). Equation L.2 and Equation L.3 are used to describe these processes, respectively.

$$\rho_{PHY(computed)} = \rho_{PHY} + \frac{0.124 \times \left(1.0 - e^{-\frac{PAR}{I_K}}\right) - 0.0230}{60} \quad (L.2)$$

$$\rho_{PHY(computed)} = \rho_{PHY} - \frac{0.0230}{60} \quad (L.3)$$

$\rho_{PHY(computed)}$ and ρ_{PHY} are the computed and initial (previous timestep) cell densities, respectively and PAR and I_K are the ambient cell photosynthetically active radiation and half saturation light intensity, respectively. I_K is specified via the light limitation function, or if not, then via the specification of the stokes settling model, or as the default. Computed cell densities are checked against specified (or default) global minima and maxima and reset to these limits if exceeded. Cell density is only used within the WQ Module to compute stokes settling, and need not be included as a computed variable if other settling models are deployed.



M Processes: organic matter

M.1 Sediment flux

Dissolved organic carbon, nitrogen and phosphorus are exchanged between the water column and sediments via specification of separate sediment fluxes. In all cases, this flux is most commonly out of the sediments, i.e. a positive specification of sediment flux. Although it is rare that sediments act as sinks of these species, TUFLOW WQ Module can be parameterised to allow for this if required. Only labile dissolved organic matter is released from the sediments in the WQ Module, and as such, references to organics in this section should be interpreted as labile organics.

The user specified rates of dissolved organic fluxes (which can be spatially varying) are modified by overlying ambient dissolved oxygen concentration (together with respective user specified half saturation oxygen concentrations) and water temperature. These modifications are simulated via Michaelis-Menten and Arrhenius models, respectively, as per Equation M.1.

$$\left. \begin{aligned} F_{sed(computed)}^{DOC} &= F_{sed}^{DOC} \times \frac{K_{sed-O_2}^{DOM}}{K_{sed-O_2}^{DOM} + [DO]} \times [\theta_{sed}^{DOM}]^{(T-20)} \\ F_{sed(computed)}^{DON} &= F_{sed}^{DON} \times \frac{K_{sed-O_2}^{DOM}}{K_{sed-O_2}^{DOM} + [DO]} \times [\theta_{sed}^{DOM}]^{(T-20)} \\ F_{sed(computed)}^{DOP} &= F_{sed}^{DOP} \times \underbrace{\frac{K_{sed-O_2}^{DOM}}{K_{sed-O_2}^{DOM} + [DO]}}_{\text{Influence of oxygen}} \times \underbrace{[\theta_{sed}^{DOM}]^{(T-20)}}_{\text{Influence of temperature}} \end{aligned} \right\} \quad (M.1)$$

F_{sed}^{DOC} , F_{sed}^{DON} and F_{sed}^{DOP} are the user specified dissolved organic carbon, nitrogen and phosphorus sediment fluxes at 20°C without the influence of dissolved oxygen, $[DO]$ is the overlying dissolved oxygen concentration, $K_{sed-O_2}^{DOM}$ is the user specified half saturation concentration of dissolved oxygen for dissolved organic matter sediment flux, θ_{sed}^{DOM} is the corresponding temperature coefficient, and T is ambient water temperature. The values of $K_{sed-O_2}^{DOM}$ and θ_{sed}^{DOM} are intentionally applied equally to dissolved organic carbon, nitrogen and phosphorus sediment fluxes. This is because there is one (not three) biological consumption process that generates these constituents: $K_{sed-O_2}^{DOM}$ and θ_{sed}^{DOM} apply to this single process. In a similar vein, the user specifications for F_{sed}^{DOC} , F_{sed}^{DON} and F_{sed}^{DOP} should not vary significantly in their relative proportions from the ratio that these typically occur in the organic matter being consumed (e.g. the Redfield ratio).

As per silicate sediment flux (see Section D.1), the above equations lead to linearly varying ambient dissolved organics concentrations in the demonstration model when dissolved oxygen concentration, half saturation oxygen concentrations and ambient temperature are set to be constant. As per FRP simulation, the above equations also lead to the form of sediment release presented in Figure F.1 and Figure F.2 when oxygen drawdown and temperature changes occur, respectively.

M.2 Hydrolysis

Hydrolysis is the pelagic biological conversion of labile particulate organic matter to labile dissolved organic matter. It is therefore a source of dissolved carbon, nitrogen and phosphorus, and a sink of the corresponding particulates. Hydrolysis neither consumes or produces dissolved oxygen or bioavailable inorganic nutrients. Hydrolysis is implemented within the labile organics constituent model of the WQ Module, and the term organic matter in this section therefore refers to labile organic matter. Refractory organic matter processes are described elsewhere.

The pelagic hydrolysis rate is computed within the labile organics constituent model via Equation M.2.

$$\left. \begin{aligned}
 R_{hyd\langle computed \rangle}^{POC} &= R_{hyd}^{POC} \times \frac{[DO]}{K_{hyd-O_2}^{POM} + [DO]} \times \underbrace{[\theta_{hyd}^{POM}]^{(T-20)}}_{\text{Influence of temperature}} \\
 R_{hyd\langle computed \rangle}^{PON} &= R_{hyd}^{PON} \times \frac{[DO]}{K_{hyd-O_2}^{POM} + [DO]} \times \underbrace{[\theta_{hyd}^{POM}]^{(T-20)}}_{\text{Influence of temperature}} \\
 R_{hyd\langle computed \rangle}^{POP} &= R_{hyd}^{POP} \times \underbrace{\frac{[DO]}{K_{hyd-O_2}^{POM} + [DO]}}_{\text{Influence of oxygen}} \times \underbrace{[\theta_{hyd}^{POM}]^{(T-20)}}_{\text{Influence of temperature}}
 \end{aligned} \right\} \quad (M.2)$$

R_{hyd}^{POC} , R_{hyd}^{PON} and R_{hyd}^{POP} are the user specified particulate organic carbon, nitrogen and phosphorus hydrolysis rates at 20°C without the influence of dissolved oxygen, $[DO]$ is the ambient dissolved oxygen concentration, $K_{hyd-O_2}^{POM}$ is the user specified half saturation concentration of dissolved oxygen for particulate organic matter hydrolysis, θ_{hyd}^{POM} is the corresponding temperature coefficient, and T is ambient water temperature. As per sediment fluxes, the values of $K_{hyd-O_2}^{POM}$ and θ_{hyd}^{POM} are intentionally applied equally to particulate organic carbon, nitrogen and phosphorus hydrolysis. This is because there is one (not three) biological consumption process that generates these constituents: $K_{hyd-O_2}^{POM}$ and θ_{hyd}^{POM} apply to this single process. In a similar vein, the user specifications for R_{hyd}^{POC} , R_{hyd}^{PON} and R_{hyd}^{POP} should not vary significantly in their relative proportions from the ratio that these typically occur in the organic matter being consumed (e.g. the Redfield ratio).

M.2.1 Consumption

The hydrolysis rates from Equation M.2 are multiplied by their respective ambient particulate organic matter concentrations to compute their respective consumptive fluxes (losses) at each model timestep in each model cell via Equation M.3.

$$\left. \begin{aligned}
 F_{hyd\langle computed \rangle}^{POC} &= R_{hyd\langle computed \rangle}^{POC} \times [POC] \\
 F_{hyd\langle computed \rangle}^{PON} &= R_{hyd\langle computed \rangle}^{PON} \times [PON] \\
 F_{hyd\langle computed \rangle}^{POP} &= R_{hyd\langle computed \rangle}^{POP} \times [POP]
 \end{aligned} \right\} \quad (M.3)$$

M.2.2 Production

The consumptive fluxes from Equation M.3 result in the dissolved organic productive fluxes in Equation M.4.

$$\left. \begin{aligned}
 F_{hyd\langle computed \rangle}^{DOC} &= F_{hyd\langle computed \rangle}^{POC} \\
 F_{hyd\langle computed \rangle}^{DON} &= F_{hyd\langle computed \rangle}^{PON} \\
 F_{hyd\langle computed \rangle}^{DOP} &= F_{hyd\langle computed \rangle}^{POP}
 \end{aligned} \right\} \quad (M.4)$$

M.3 Breakdown

Breakdown is the pelagic biological conversion of refractory particulate organic matter (which is a single computed variable) to three labile particulate organic matter computed variables. It is therefore a source of labile particulate organic carbon, nitrogen and phosphorus, and a sink of refractory particulate organic matter. Breakdown neither consumes or produces dissolved oxygen or bioavailable inorganic nutrients. Breakdown is implemented within the

refractory organics constituent model of the WQ Module only, so the following does not apply if the labile organics constituent model is used.

The pelagic breakdown rate of refractory particulate organic matter is computed via Equation M.5.

$$R_{bdn\langle computed \rangle}^{RPOM} = R_{bdn}^{RPOM} \times \underbrace{\frac{[DO]}{K_{hyd-O_2}^{POM} + [DO]}}_{\text{Influence of oxygen}} \times \underbrace{[\theta_{hyd}^{POM}]^{(T-20)}}_{\text{Influence of temperature}} \quad (M.5)$$

R_{bdn}^{RPOM} is the user specified (or default) refractory particulate organic matter breakdown rate at 20°C without the influence of dissolved oxygen, $[DO]$ is the ambient dissolved oxygen concentration, $K_{hyd-O_2}^{POM}$ is the user specified (or default) half saturation concentration of dissolved oxygen for labile particulate organic matter hydrolysis, θ_{hyd}^{POM} is the corresponding temperature coefficient, and T is ambient water temperature. The parameters $K_{hyd-O_2}^{POM}$ and θ_{hyd}^{POM} used in Equation M.5 are the same as those used for the hydrolysis calculations described in Section M.2 and specified via the associated labile organic matter hydrolysis command.

M.3.1 Consumption

The breakdown rate from Equation M.5 is multiplied by the ambient refractory particulate organic matter concentration to compute its consumptive flux (loss) at each model timestep in each model cell via Equation M.6.

$$F_{bdn\langle computed \rangle}^{RPOM} = R_{bdn\langle computed \rangle}^{RPOM} \times [RPOM] \quad (M.6)$$

M.3.2 Production

The consumptive flux from Equation M.6 results in the labile particulate organic carbon, nitrogen and phosphorus productive fluxes in Equation M.7.

$$\left. \begin{aligned} F_{bdn\langle computed \rangle}^{POC} &= F_{bdn\langle computed \rangle}^{RPOM} \\ F_{bdn\langle computed \rangle}^{PON} &= F_{bdn\langle computed \rangle}^{RPOM} \times X_N^{RPOM} \\ F_{bdn\langle computed \rangle}^{POP} &= F_{bdn\langle computed \rangle}^{RPOM} \times X_P^{RPOM} \end{aligned} \right\} \quad (M.7)$$

X_N^{RPOM} and X_P^{RPOM} are the user specified (or default) molar ratios of nitrogen and phosphorus to carbon within refractory particulate organic matter. These should not differ significantly from the Redfield ratios of 16/106 and 1/106, respectively.

M.4 Mineralisation

Mineralisation is the pelagic biological conversion of labile dissolved organic matter to dissolved inorganic carbon and nutrients. It is therefore a source of dissolved inorganic carbon, ammonium and filterable reactive phosphorus, and a sink of the corresponding labile dissolved organics. Mineralisation is conceptualised as comprising aerobic (i.e. consuming dissolved oxygen and (via denitrification) inorganic nitrate) and anaerobic components, and is implemented within the labile organics constituent model of the WQ Module. The term organic matter in this section therefore refers to labile organic matter.

The same pelagic mineralisation rate is computed within the WQ Module for dissolved organic carbon, nitrogen and phosphorus via Equation M.8.

$$R_{miner\langle computed \rangle}^{DOM} = R_{miner}^{DOM} \times \underbrace{\left[\underbrace{\frac{[DO]}{K_{miner-O_2}^{DOM} + [DO]}}_{\text{O2 consumption}} + f_{an} \times \underbrace{\frac{K_{miner-O_2}^{DOM}}{K_{miner-O_2}^{DOM} + [DO]}}_{\text{non-O2 consumption}} \right]}_{\text{Influence of oxygen}} \times \underbrace{[\theta_{miner}^{DOM}]^{(T-20)}}_{\text{Influence of temperature}} \quad (M.8)$$

R_{miner}^{DOM} is the user specified (or default) dissolved organic matter (i.e. carbon, nitrogen and phosphorus) mineralisation rate at 20°C without the influence of dissolved oxygen, $[DO]$ is the ambient dissolved oxygen concentration, $K_{miner-O_2}^{DOM}$ is the user specified half saturation concentration of dissolved oxygen for dissolved organic matter mineralisation, θ_{miner}^{DOM} is the corresponding temperature coefficient, f_{an} is a fractional multiplier that weights the Michaelis-Menten contribution of non-O₂ processes within the calculation of total mineralisation and T is ambient water temperature. As per sediment fluxes and hydrolysis, the values of $K_{miner-O_2}^{DOM}$ and θ_{miner}^{DOM} are intentionally applied equally to dissolved organic carbon, nitrogen and phosphorus mineralisation. In addition, the rate at which mineralisation of dissolved organic matter (to inorganics) occurs is the same for all dissolved organic constituents. This is because there is one (not three) biological conversion process that is assumed to draw equally on all dissolved organic constituents. Finally, setting f_{an} to zero does not suppress entirely non-O₂ mineralisation (see following section), but it does remove the Michaelis-Menten based influence of anaerobic processes on the calculation of total mineralisation.

M.4.1 Consumption

The mineralisation rate from Equation M.8 is multiplied by ambient labile dissolved organic carbon, nitrogen and phosphorus concentrations to compute their respective consumptive fluxes (losses) at each model timestep in each model cell via Equation M.9.

$$\left. \begin{aligned} F_{miner\langle computed \rangle}^{DOC} &= R_{miner\langle computed \rangle}^{DOM} \times [DOC] \\ F_{miner\langle computed \rangle}^{DON} &= R_{miner\langle computed \rangle}^{DOM} \times [DON] \\ F_{miner\langle computed \rangle}^{DOP} &= R_{miner\langle computed \rangle}^{DOM} \times [DOP] \end{aligned} \right\} \quad (M.9)$$

The fraction of dissolved organic carbon mineralisation that consumes dissolved oxygen O₂ is given by Equation M.10. $K_{miner-O_2}^{DOM}$, $[DO]$ and f_{an} have been described previously.

$$f_{miner-O_2\langle computed \rangle}^{DOC} = \frac{\frac{[DO]}{K_{miner-O_2}^{DOM} + [DO]}}{\frac{[DO]}{K_{miner-O_2}^{DOM} + [DO]} + f_{an} \times \frac{K_{miner-O_2}^{DOM}}{K_{miner-O_2}^{DOM} + [DO]}} \quad (M.10)$$

Applying a 1:1 molar ratio of mineralised dissolved organic carbon to consumed diatomic dissolved oxygen, gives the consumptive oxygen flux $F_{miner\langle computed \rangle}^{O_2}$ as:

$$F_{miner\langle computed \rangle}^{O_2} = F_{miner\langle computed \rangle}^{DOC} \times f_{miner-O_2\langle computed \rangle}^{DOC} \quad (M.11)$$

Substituting Equation M.8 and Equation M.9 into Equation M.11 and cancelling terms gives the final expression for $F_{miner\langle computed \rangle}^{O_2}$ as Equation M.12, again with parameters described previously.

$$F_{miner\langle computed \rangle}^{O_2} = F_{miner\langle computed \rangle}^{DOC} \times \frac{[DO]}{K_{miner-O_2}^{DOM} + [DO]} \quad (M.12)$$

This is also expressed as the reduction of ambient dissolved oxygen concentration that would result from this consumptive mineralisation over a period of five days. It is a common laboratory reporting unit and referred to as BOD5 (biological oxygen demand over 5 days). BOD5 is computed as per Equation M.13.

$$BOD5_{miner\langle computed \rangle}^{O_2} = F_{miner\langle computed \rangle}^{O_2} \times 5 \quad (M.13)$$

A portion of remaining mineralisation ($F_{miner\langle computed \rangle}^{DOC} - F_{miner\langle computed \rangle}^{O_2}$) flux (that follows dissolved oxygen consumption) sources its oxygen from ambient nitrate. This consumptive flux of nitrate $F_{miner\langle computed \rangle}^{NO_3}$ is referred to as denitrification and is the reduction of nitrate N to free diatomic nitrogen gas. Again applying a 1:1 molar ratio of consumed dissolved organic carbon to nitrate, this quantity is computed via Equation M.14.

$$F_{miner\langle computed \rangle}^{NO_3} = (F_{miner\langle computed \rangle}^{DOC} - F_{miner\langle computed \rangle}^{O_2}) \times \frac{[NO_3]}{K_{miner-NO_3}^{NO_3} + [NO_3]} \quad (M.14)$$

$K_{miner-NO_3}^{NO_3}$ is the user specified half saturation concentration of nitrate for consumption of nitrate as result of mineralisation of dissolved organic carbon and $[NO_3]$ is the ambient nitrate concentration.

The remaining dissolved organic carbon mineralisation flux is referred to as anaerobic mineralisation, $F_{miner\langle computed \rangle}^{an}$, such that the following overall molar equality applies (with O_2 and NO_3 being in a 1:1 molar ration with their respective carbon fluxes):

$$F_{miner\langle computed \rangle}^{DOC} = F_{miner\langle computed \rangle}^{O_2} + F_{miner\langle computed \rangle}^{NO_3} + F_{miner\langle computed \rangle}^{an} \quad (M.15)$$

In summary:

- $F_{miner\langle computed \rangle}^{DOC}$ is the total mineralisation flux of DOC to dissolved inorganics
- $F_{miner\langle computed \rangle}^{O_2}$ is the portion of the total mineralisation flux that uses dissolved oxygen as its oxygen source. The flux of DOC and dissolved oxygen are applied as a 1:1 molar ratio
- $F_{miner\langle computed \rangle}^{NO_3}$ is the portion of the total mineralisation flux that uses nitrate as its oxygen source. The flux of DOC and nitrate are applied as a 1:1 molar ratio
- $F_{miner\langle computed \rangle}^{an}$ is the remaining portion of the total mineralisation flux that uses no oxygen. It consumes no computed variables other than DOC

All these mineralisation diagnostic variables are reported in units of carbon.

M.4.2 Production

The consumptive flux from Equation M.6 results in the inorganic carbon, ammonium and FRP productive fluxes in Equation M.16.

$$\left. \begin{aligned} F_{miner\langle computed \rangle}^{DIC} &= F_{miner\langle computed \rangle}^{DOC} \\ F_{miner\langle computed \rangle}^{NH_4} &= F_{miner\langle computed \rangle}^{DON} \\ F_{miner\langle computed \rangle}^{FRP} &= F_{miner\langle computed \rangle}^{DOP} \end{aligned} \right\} \quad (M.16)$$

The WQ Module does not currently support simulation of dissolved inorganic carbon (DIC) so the corresponding carbonic productive flux in Equation M.16 has no effect on inorganic water quality dynamics. Contact support@tufLOW.com if the DIC model is required.

M.5 Activation

Activation is the pelagic biological conversion of refractory dissolved organic carbon, nitrogen and phosphorus to their respective labile dissolved organic equivalents. It is therefore a source of dissolved labile organic carbon, nitrogen and phosphorus, and a sink of the corresponding refractory dissolved organics. Activation does not consume or produce any other computed variables, although its computed rate does depend on dissolved oxygen concentration.

The pelagic activation rate is computed within the WQ Module for refractory dissolved organic carbon, nitrogen and phosphorus via Equation M.17.

$$R_{act(computed)}^{RDOM} = R_{act}^{RDOM} \times \underbrace{\left[\underbrace{\frac{[DO]}{K_{miner-O_2}^{DOM} + [DO]}}_{\text{aerobic}} + f_{an} \times \underbrace{\frac{K_{miner-O_2}^{DOM}}{K_{miner-O_2}^{DOM} + [DO]}}_{\text{anaerobic}} \right]}_{\text{Influence of oxygen}} \times \underbrace{[\theta_{miner}^{DOM}]^{(T-20)}}_{\text{Influence of temperature}} \quad (M.17)$$

R_{act}^{RDOM} is the user specified refractory dissolved organic matter (i.e. carbon, nitrogen and phosphorus) activation rate at 20°C without the influence of dissolved oxygen, $[DO]$ is the ambient dissolved oxygen concentration, $K_{miner-O_2}^{DOM}$ is the user specified half saturation concentration of dissolved oxygen for dissolved organic matter mineralisation, θ_{miner}^{DOM} is the corresponding temperature coefficient, f_{an} is a fractional multiplier that weights the Michaelis-Menten contribution of non- O_2 processes within the calculation of total mineralisation and T is ambient water temperature. The parameters $K_{miner-O_2}^{DOM}$, f_{an} and θ_{miner}^{DOM} used in Equation M.17 are the same as those used for the mineralisation calculations described in Section M.4 and specified via the associated labile organic matter mineralisation command. If this is the case and labile organic matter mineralisation is not required as a simulated process, then the command can still be issued but with the first argument, R_{miner}^{DOM} , equal to zero.

M.5.1 Consumption

The activation rate from Equation M.17 is multiplied by the ambient refractory dissolved carbon, nitrogen and phosphorus concentrations to compute their respective consumptive fluxes (losses) at each model timestep in each model cell via Equation M.18.

$$\left. \begin{aligned} F_{act(computed)}^{RDOC} &= R_{act(computed)}^{RDOM} \times [RDOC] \\ F_{act(computed)}^{RDON} &= R_{act(computed)}^{RDOM} \times [RDON] \\ F_{act(computed)}^{RDOP} &= R_{act(computed)}^{RDOM} \times [RDOP] \end{aligned} \right\} \quad (M.18)$$

M.5.2 Production

The consumptive flux from Equation M.18 results in the labile dissolved organic carbon, nitrogen and phosphorus productive fluxes in Equation M.19.

$$\left. \begin{aligned} F_{act(computed)}^{DOC} &= F_{act(computed)}^{RDOC} \\ F_{act(computed)}^{DON} &= F_{act(computed)}^{RDON} \\ F_{act(computed)}^{DOP} &= F_{act(computed)}^{RDOP} \end{aligned} \right\} \quad (M.19)$$

M.6 Photolysis

The WQ Module conceptualises photolysis as the conversion of refractory dissolved organic carbon, nitrogen and phosphorus to their labile dissolved and inorganic equivalents, under the action of photosynthetically active (PAR), ultraviolet A (UVA) and ultraviolet B (UVB) radiation. These radiation bands are provided to the WQ Module from TUFLOW for each computational cell at each water quality timestep. The WQ Module computes total photolysis of refractory dissolved organic carbon $F_{photo-tot}^{RDOC}$ as the sum of photolysis due to each of these three bands via Equation M.20.

$$F_{photo-tot}^{RDOC} = F_{photo-PAR}^{RDOC} + F_{photo-UVA}^{RDOC} + F_{photo-UVB}^{RDOC} \quad (M.20)$$

Each band's photolysis is computed via Equation M.21, with Radiation_{band} (where band is PAR, UVA or UVB) being previously converted from W/m^2 (as provided by TUFLOW) to moles of photons.

$$F_{photo-band}^{RDOC} = \text{Radiation}_{band} \times \underbrace{c \times 10^{-d \times \lambda_{band}}}_{\text{Apparent quantum yield}} \times \underbrace{CDOM \times e^{S \times (x - \lambda_{band})}}_{\text{Absorption coefficient}} \quad (\text{M.21})$$

where $c = 7.52$, $d = 0.0122$, λ_{band} is each band's characteristic wavelength, $S = 0.0188$ and $x = 440.0$ nm. $CDOM$ is chromomorphically dissolved organic matter and is computed via Equation M.22.

$$CDOM_{(computed)} = 0.35 \times e^{0.1922 \times ([DOC] + [RDOC]) \times (12/1000)} \quad (\text{M.22})$$

$[DOC]$ and $[RDOC]$ and the ambient concentrations of labile and refractory dissolved organic carbon, respectively.

M.6.1 Consumption

Once total photolysis has been computed, the associated consumptive fluxes (losses) of refractory dissolved organic carbon, nitrogen and phosphorus are computed via Equation M.23, using ambient refractory dissolved nitrogen and phosphorus concentrations to proportion the computed fluxes.

$$\left. \begin{aligned} F_{photo(computed)}^{RDOC} &= F_{photo-tot}^{RDOC} \\ F_{photo(computed)}^{RDON} &= F_{photo-tot}^{RDOC} \times \frac{[RDON]}{[RDOC]} \\ F_{photo(computed)}^{RDOP} &= F_{photo-tot}^{RDOC} \times \frac{[RDOP]}{[RDOC]} \end{aligned} \right\} \quad (\text{M.23})$$

M.6.2 Production

The consumptive fluxes from Equation M.23 result in the labile dissolved organic carbon, nitrogen and phosphorus productive fluxes in Equation M.24.

$$\left. \begin{aligned} F_{photo(computed)}^{DOC} &= F_{photo(computed)}^{RDOC} \times f_{photo}^{RDOM} \\ F_{photo(computed)}^{DON} &= F_{photo(computed)}^{RDON} \times f_{photo}^{RDOM} \\ F_{photo(computed)}^{DOP} &= F_{photo(computed)}^{RDOP} \times f_{photo}^{RDOM} \end{aligned} \right\} \quad (\text{M.24})$$

f_{photo}^{RDOM} is the proportion of the total photolysed refractory dissolved organic matter that becomes the corresponding labile organics. The remainder of the photolysed refractory dissolved organic matter fluxes produce inorganic carbon and nutrients via Equation M.25.

$$\left. \begin{aligned} F_{photo(computed)}^{DIC} &= F_{photo(computed)}^{RDOC} \times (1.0 - f_{photo}^{RDOM}) \\ F_{photo(computed)}^{NH_4} &= F_{photo(computed)}^{RDON} \times (1.0 - f_{photo}^{RDOM}) \\ F_{photo(computed)}^{FRP} &= F_{photo(computed)}^{RDOP} \times (1.0 - f_{photo}^{RDOM}) \end{aligned} \right\} \quad (\text{M.25})$$

The WQ Module does not currently support simulation of dissolved inorganic carbon (DIC) so the corresponding carbonic productive flux in Equation M.25 has no effect on inorganic water quality dynamics. Contact support@tufLOW.com if the DIC model is required.

M.7 Self shading

Photosynthetically available radiation is provided to the WQ Module from TUFLOW for each computational cell at each water quality timestep. The WQ Module allows for modification of this TUFLOW field to incorporate the effect of light attenuation due to the presence of particulate and dissolved organic matter. This additional light extinction is computed dynamically at each water quality timestep, based on instantaneous organic matter concentrations in individual computational cells.

For labile organics, the associated additive specific light attenuation coefficient is computed as per Equation M.26.

$$K_{e_{(computed)}}^{OM} = K_e^{POM} \times [POC] + K_e^{DOM} \times [DOC] \quad (M.26)$$

K_e^{POM} and K_e^{DOM} are the user specified (or default) specific shading coefficients for labile particulate and dissolved organic matter respectively, and $[POC]$ and $[DOC]$ are the ambient labile particulate and dissolved organic carbon concentrations (used as proxies for organic matter) in each cell. For each cell and at each timestep, this quantity $K_{e_{(computed)}}^{OM}$ is computed and returned to TUFLOW as a two- or three-dimensional field which TUFLOW then includes these in subsequent light distribution calculations.

For refractory organics (if computed), the associated additive specific light attenuation coefficient is computed as per Equation M.27.

$$K_{e_{(computed)}}^{ROM} = R_{CDOM}^{RDOM} \times CDOM + K_e^{RPOM} \times [RPOM] \quad (M.27)$$

R_{CDOM}^{RDOM} is a user specified (or default) dimensionless multiplier applied to the CDOM computed in Equation M.22, where the same CDOM is used in photolysis calculations. R_{CDOM}^{RDOM} is not a specific shading coefficient, but can be thought of as (light attenuation (/m) / CDOM (/m)), or the strength of CDOM in attenuating light. K_e^{RPOM} is the user specified (or default) specific shading coefficient for refractory particulate organic matter, and $[RPOM]$ is the instantaneous refractory particulate organic matter concentration in each cell. For each cell and at each timestep, this quantity $K_{e_{(computed)}}^{ROM}$ is computed and returned to TUFLOW as a two- or three-dimensional field which TUFLOW then includes these in subsequent light distribution calculations.

M.8 Settling

Particulate organic matter is able to be settled within the WQ Module. Four settling models are available. These are able to be applied equally to both labile and refractory particulate organic matter to compute V_{settle}^{long} and V_{settle}^{rorg} , respectively. The same settling model must be applied to both types of particulates, although the parameters ascribed to a model can be different for labile and refractory particulates. Once computed, the same settling rate is applied to each of labile particulate organic carbon, nitrogen and phosphorus.

M.8.1 None

In this model, particulate organic settling is set to zero and organic matter is simply advected by the hydrodynamic flow field.

M.8.2 Constant

In this model, V_{settle}^{long} and V_{settle}^{rorg} are set to constant values, and matter is settled at these velocities. These can be different velocities for labile and refractory particulate organics. A negative specification of this quantity corresponds to a downwards settling velocity.

M.8.3 Constant with density correction

In this model, V_{settle}^{long} and V_{settle}^{rorg} are set to constant values, and matter is settled at these velocities, but corrected for ambient water density effects, as per Equation M.28.

$$V_{sett(computed)}^{org} = V_{settle}^{org} \times \frac{\mu_{20} \times \rho_w}{\mu \times \rho_{w20}} \quad (M.28)$$

V_{settle}^{org} is V_{settle}^{lorg} or V_{settle}^{rorg} at 20°C, μ and ρ_w are the ambient water dynamic viscosity (in Ns/m²) and density (in kg/m³), respectively, and μ_{20} and ρ_{w20} are the dynamic viscosity and density of freshwater at 20°C, respectively. A negative specification of V_{settle}^{org} corresponds to a downwards settling velocity.

M.8.4 Stokes

In this model, particulate organic settling is computed using the Stokes equation and particle diameter and density, as per Equation M.29 and Equation M.30.

$$V_{sett(computed)}^{lorg} = -g \times d_{lorg}^2 \times \frac{(\rho_{lorg} - \rho_w)}{18\mu} \quad (M.29)$$

$$V_{sett(computed)}^{rorg} = -g \times d_{rorg}^2 \times \frac{(\rho_{rorg} - \rho_w)}{18\mu} \quad (M.30)$$

g is acceleration due to gravity, d_{lorg} and d_{rorg} are conceptualised diameters of labile and refractory particulate organic matter respectively, ρ_{lorg} and ρ_{rorg} are labile and refractory particulate organic matter densities, respectively, and ρ_w and μ are the ambient water density and dynamic viscosity, respectively.

Once the settling velocities for labile and refractory particulate organic matter have been computed, the relevant fluxes are calculated as follows.

$$\left. \begin{aligned} F_{sedmnt(computed)}^{POC} &= (V_{sett(computed)}^{lorg}/dz) \times [POC] \\ F_{sedmnt(computed)}^{PON} &= (V_{sett(computed)}^{lorg}/dz) \times [PON] \\ F_{sedmnt(computed)}^{POP} &= (V_{sett(computed)}^{lorg}/dz) \times [POP] \end{aligned} \right\} \quad (M.31)$$

$$F_{sedmnt(computed)}^{RPOM} = (V_{sett(computed)}^{rorg}/dz) \times [RPOM] \quad (M.32)$$

dz is the relevant cell thickness, and divides the flux to produce a per volume result for consistency with other corresponding diagnostics.

The limitations of this approach to modelling particulate organic matter settling are recognised. Future releases of the WQ Module will offer direct linkages between the TUFLOW FV ST Module and WQ Module, and treat particulate organics as sediment fractions that are transported using the advanced techniques and models offered by the ST Module.

N Processes: pathogens

N.1 Mortality

Natural mortality, or the ‘dark-death rate’ k_d^{pth} is an important process influencing protozoan, bacterial and viral dynamics in surface and coastal waters. Two of the predominant environmental factors known to modify this dark death rate are temperature and salinity, and as such the resultant mortality flux is computed via Equation N.1.

$$F_{mor}^{pth} = [k_d^{pth} + C_{SM}^{pth} \times S^\alpha] \times [\theta_{mor}^{pth}]^{T-20} \times ([PTH_a] + [PTH_t]) \quad (N.1)$$

k_d^{pth} is the user specified dark death rate in freshwater at 20°C, C_{SM}^{pth} is the salinity effect on mortality, S is ambient salinity, α is a parameter controlling salinity dependence, θ_{mor}^{pth} is the corresponding temperature coefficient, T is ambient water temperature, and $[PTH_a]$ and $[PTH_t]$ are the concentrations of free and attached pathogens, respectively. If attached pathogens are not simulated, then the latter concentration is set to zero for the purposes of the above flux calculation.

N.2 Inactivation

Sunlight exposure is an important inactivation mechanism for all forms of pathogens and microbial indicators in both fresh and saline waters. In waters of high clarity, it has long been regarded as the most dominant inactivation mechanism. To compute this inactivation flux, the individual inactivation rates due to visible, UVA and UVB light are calculated and combined to compute an overall inactivation rate R_{invn}^{pth} via Equation N.2.

$$R_{invn}^{pth} = 10^{-6} \times \left(\underbrace{\left[\frac{[DO]}{K_{DO_{vis}}^{pth} + [DO]} \times [k_{vis}^{pth} + c_{S_{vis}}^{pth} S] \times PAR \right]}_{\text{Influence of visible light}} + \dots \underbrace{\left[\frac{[DO]}{K_{DO_{uva}}^{pth} + [DO]} \times [k_{uva}^{pth} + c_{S_{uva}}^{pth} S] \times UVA \right]}_{\text{Influence of UV-A light}} + \dots \left[\frac{[DO]}{K_{DO_{uvb}}^{pth} + [DO]} \times [k_{uvb}^{pth} + c_{S_{uvb}}^{pth} S] \times UVB \right] \right) \quad (N.2)$$

$K_{DO_{vis}}^{pth}$, $K_{DO_{uva}}^{pth}$, and $K_{DO_{uvb}}^{pth}$ are the user specified half saturation oxygen concentrations for visible, UV-A and UV-B light inactivation, respectively, k_{vis}^{pth} , k_{uva}^{pth} , and k_{uvb}^{pth} are the user specified freshwater inactivation rate coefficients for exposure to visible, UV-A and UV-B light, respectively, $c_{S_{vis}}^{pth}$, $c_{S_{uva}}^{pth}$, and $c_{S_{uvb}}^{pth}$ are the user specified coefficients that enhance the inactivation effect of light under saline conditions for exposure to visible, UV-A and UV-B light, respectively, S is ambient salinity, and PAR , UVA and UVB are the photosynthetically available, UV-A and UV-B radiation intensities at the centre of a model cell. The multiplier preceding the calculation is for units conversion purposes.

The inactivation rate R_{invn}^{pth} from Equation N.2 is multiplied by free and attached pathogen concentrations to compute the inactivation flux at each model timestep in each model cell via Equation N.3.

$$F_{invn}^{pth} = R_{invn}^{pth} \times \left([PTH_a] + \frac{[PTH_t]}{2} \right) \quad (N.3)$$

$[PTH_a]$ and $[PTH_t]$ are the concentrations of free and attached pathogens, respectively. If attached pathogens are not simulated then $[PTH_t]$ is set to zero for the purposes of the above calculation. The reduced (50%) impact of R_{invn}^{pth} on attached pathogens reflects the shading of half of all attached pathogens by their associated sediment particles (i.e. those on the underside).

N.3 Attachment

Enteric organisms may exist in isolation or be associated with either organic or inorganic suspended particles, depending on the surface properties of the organism and the nature of the suspended material within the system. The simulation of this attachment (and detachment) is therefore allowed for within the TUFLOW WQ Module as an attachment to total suspended sediment.

At each water quality timestep, the instantaneous attachment flux F_{att}^{pth} is estimated via Equation N.4.

$$F_{att}^{pth} = \frac{1}{7} \times \left(f_{att}^{pth} \times ([PTH_a] + [PTH_t]) - [PTH_a] \right) \quad (N.4)$$

f_{att}^{pth} is the user specified target attachment fraction, and $[PTH_a]$ and $[PTH_t]$ are the concentrations of free and attached pathogens, respectively. This assumes that left unperturbed, equilibrium would be reached in seven days. A positive (negative) flux represents attachment (detachment). The target attachment fraction is defined as follows, where the concentrations are relative targets, not actual simulated quantities (i.e. so cannot be algebraically cancelled if the expression for f_{att}^{pth} in Equation N.5 is substituted into Equation N.4).

$$f_{att}^{pth} = \frac{[PTH_a]}{[PTH_a] + [PTH_t]} \quad (N.5)$$

N.4 Settling

Unattached pathogens able to be settled within the WQ Module, at a user specified constant settling velocity, V_{settle}^{pth} . This is applied equally to both unattached alive and unattached dead pathogens, and a negative velocity is downwards settling. The relevant fluxes are then calculated as follows.

$$\left. \begin{aligned} F_{sedmntn(computed)}^{pth_a} &= \frac{V_{settle}^{pth}}{dz} \times [PTH_a] \\ F_{sedmntn(computed)}^{pth_d} &= \frac{V_{settle}^{pth}}{dz} \times [PTH_d] \end{aligned} \right\} \quad (N.6)$$

V_{settle}^{pth} is the user specified settling velocity and dz is the relevant cell thickness. The latter divides the flux to produce a per volume result for consistency with other corresponding diagnostics. $[PTH_a]$ and $[PTH_d]$ are the concentrations of unattached alive and dead pathogens, respectively. Settled pathogens are not permitted to resuspend.

If attached pathogens are simulated, then their settling velocity $V_{settle}^{pth_t}$ is also specified as a constant (with a negative value again being downwards). This specification should be comparable to the settling velocity/ies specified in the TUFLOW FV Sediment Transport Module configuration. The relevant flux is then calculated as follows.

$$F_{sedmntn(computed)}^{pth_t} = \frac{V_{settle}^{pth_t}}{dz} \times [PTH_t] \quad (N.7)$$

The limitations of the above approaches to modelling pathogenic settling are recognised. Future releases of the WQ Module will offer direct linkages between the TUFLOW FV ST Module and WQ Module, and treat pathogens as sediment fractions that are transported using the advanced techniques and models offered by the ST Module, including resuspension.

N.5 Other

N.5.1 Total pathogens

Total pathogens is reported as a diagnostic variable computed as per Equation N.8

$$[PTH]^{TOT} = [PTH_a] + [PTH_d] + [PTH_t] \quad (N.8)$$

$[PTH_a]$, $[PTH_d]$ and $[PTH_t]$ are the concentrations of free, dead and attached pathogens, respectively.

O Computed variables

O.1 Overview

The WQ Module's computed variables, and the core (lowest order) constituent model class and instance where each is deployed are listed below ([Computed Variables](#)). Output variable names are also included for cross referencing. Some TUFLOW FV variables are included for completeness.

Each computed variable entry comprises the following components:

- Computed variable heading: The variable symbol in mathematical notation and its full descriptive name.
- Output variable name: Exact string to use in TUFLOW FV output blocks when requesting this variable (see Section [O.1.1](#)). Where both unit systems are supported, variable names and units for both systems are listed in a table. See [Unit Systems](#) for more information on the unit systems.
- Units: The units for the computed variable. Where both unit systems are supported, units are shown as outlined above.
- Relevant Element, Atomic Number (Z) and Atomic Weight (M): Where applicable, these identify the element in which concentrations are reported. See [Concentration Nomenclature](#) for further detail.
- Core Constituent Model: Where applicable, this links to the core constituent model for the computed variable. See Section [2.2.3](#) for details on the available constituent models.

O.1.1 Computed Variable Naming

Below are some key points with regard to naming of computed variables:

- The text NAME in variable names is a placeholder for the user defined phytoplankton group name.
For example, `WQ-PHYTO-NAME-INT-N-MG-L` would be named `WQ-PHYTO-CYLINDRO-INT-N-MG-L` if a user defined phytoplankton group name was `cylindro`

- The **TUFLOW FV MATLAB toolbox**:
 - Offers several post processing tools which rely on output phytoplankton group names. These are defined in `..\TUFLOWFV_Matlab_Utillities_001\toolbox\tuflowfv\fv_variables.m` with default names: `BLUEGREEN`, `BGA`, `FDIAT`, `MDIAT`, `DIATOM`, `GREEN`, `PHY01`, `PHY02`, `PHY03`, `PHY04`, `PHY05`, `PHY06`, `PHY07`, `PHY08`, `PHY09`, `PHY10` and `PHY11`. Users may choose to deploy any of these names and therefore use the MATLAB post processing tools unchanged. If not, then users will need to extend the `fvwq_mgL` or `fvwq_mmm` name lists provided in `fv_variables.m`. A template is provided in that mfile, with instructions on what to change.
 - Uses dissolved oxygen in the following example scripts. It has been assumed that the MGL units system has been used so that the variable name of the interrogated data set is `WQ-DISS-OXYGEN-MG-L`. Users can change this if desired. Other ancillaries such as plot labels, colour limits and scale factors will also need to be changed for correct presentation of data if oxygen in the MGL units system is not processed:
 - * `..\TUFLOWFV_Matlab_Utillities_001\tutorial\visual\3.sheets\sh_006_impact_sheet_multiple`
 - * `..\TUFLOWFV_Matlab_Utillities_001\tutorial\visual\4.curtains\cu_000_plot_curtain_WQ.m`
 - * `..\TUFLOWFV_Matlab_Utillities_001\tutorial\visual\5.combined_plots\co_000_plot_multiple`
- Output computed variable names are exact, and can therefore be copied and pasted directly into output blocks of control files. The exception is phytoplankton variables, where the user specified group name is included within the variable name, so will need to be inserted by the user.

O.2 Computed Variables

$[DO]$ - Dissolved Oxygen

Units	Output Variable Name
mg/L	WQ DISS_OXYGEN_MG_L
mmol/m ³	WQ DISS_OXYGEN_MM_M3

Relevant Element: O_2
Atomic Number (Z): 16
Atomic Weight (M): 32
Core Constituent Model: [Oxygen - O2](#)

 $[Si]$ - Silicate

Units	Output Variable Name
mg/L	WQ SILICATE_MG_L
mmol/m ³	WQ SILICATE_MM_M3

Relevant Element: Si
Atomic Number (Z): 14
Atomic Weight (M): 28
Core Constituent Model: [Silicate - Si](#)

 $[NH_4]$ - Ammonium

Units	Output Variable Name
mg/L	WQ AMMONIUM_MG_L
mmol/m ³	WQ AMMONIUM_MM_M3

Relevant Element: N
Atomic Number (Z): 7
Atomic Weight (M): 14
Core Constituent Model: [Inorganic nitrogen - AmoniumNitrate](#)

 $[NO_3]$ - Nitrate

Units	Output Variable Name
mg/L	WQ NITRATE_MG_L
mmol/m ³	WQ NITRATE_MM_M3

Relevant Element: N
Atomic Number (Z): 7
Atomic Weight (M): 14
Core Constituent Model: [Inorganic nitrogen - AmoniumNitrate](#)

[FRP] - Filterable Reactive Phosphorus

Units	Output Variable Name
mg/L	WQ_FRP_MG_L
mmol/m ³	WQ_FRP_MM_M3

Relevant Element: *P*
Atomic Number (Z): 15
Atomic Weight (M): 31
Core Constituent Model: [Inorganic phosphorus - FRPhs](#)

[FRPads] - Filterable Reactive Phosphorus Adsorbed

Units	Output Variable Name
mg/L	WQ_FRP_ADS_MG_L
mmol/m ³	WQ_FRP_ADS_MM_M3

Relevant Element: *P*
Atomic Number (Z): 15
Atomic Weight (M): 31
Core Constituent Model: [Inorganic phosphorus - FRPhsads](#)

[DOC] - Dissolved Organic Carbon

Units	Output Variable Name
mg/L	WQ_DOC_MG_L
mmol/m ³	WQ_DOC_MM_M3

Relevant Element: *C*
Atomic Number (Z): 6
Atomic Weight (M): 12
Core Constituent Model: [Organic matter - Labile](#)

[POC] - Particulate Organic Carbon

Units	Output Variable Name
mg/L	WQ_POC_MG_L
mmol/m ³	WQ_POC_MM_M3

Relevant Element: *C*
Atomic Number (Z): 6
Atomic Weight (M): 12
Core Constituent Model: [Organic matter - Labile](#)

[DON] - Dissolved Organic Nitrogen

Units	Output Variable Name
mg/L	WQ_DON_MG_L
mmol/m ³	WQ_DON_MM_M3

Relevant Element: *N*
Atomic Number (Z): 7
Atomic Weight (M): 14
Core Constituent Model: [Organic matter - Labile](#)

[PON] - Particulate Organic Nitrogen

Units	Output Variable Name
mg/L	WQ_PON_MG_L
mmol/m ³	WQ_PON_MM_M3

Relevant Element: *N*
Atomic Number (Z): 7
Atomic Weight (M): 14
Core Constituent Model: [Organic matter - Labile](#)

[DOP] - Dissolved Organic Phosphorus

Units	Output Variable Name
mg/L	WQ_DOP_MG_L
mmol/m ³	WQ_DOP_MM_M3

Relevant Element: *P*
Atomic Number (Z): 15
Atomic Weight (M): 31
Core Constituent Model: [Organic matter - Labile](#)

[POP] - Particulate Organic Phosphorus

Units	Output Variable Name
mg/L	WQ_POP_MG_L
mmol/m ³	WQ_POP_MM_M3

Relevant Element: *P*
Atomic Number (Z): 15
Atomic Weight (M): 31
Core Constituent Model: [Organic matter - Labile](#)

[*RDOC*] – Refractory Dissolved Organic Carbon

Units	Output Variable Name
mg/L	WQ_RDOC_MG_L
mmol/m ³	WQ_RDOC_MM_M3

Relevant Element: *C*
Atomic Number (Z): 6
Atomic Weight (M): 12
Core Constituent Model: [Organic matter - Refractory](#)

[*RDON*] – Refractory Dissolved Organic Nitrogen

Units	Output Variable Name
mg/L	WQ_RDON_MG_L
mmol/m ³	WQ_RDON_MM_M3

Relevant Element: *N*
Atomic Number (Z): 7
Atomic Weight (M): 14
Core Constituent Model: [Organic matter - Refractory](#)

[*RDOP*] – Refractory Dissolved Organic Phosphorus

Units	Output Variable Name
mg/L	WQ_RDOP_MG_L
mmol/m ³	WQ_RDOP_MM_M3

Relevant Element: *P*
Atomic Number (Z): 15
Atomic Weight (M): 31
Core Constituent Model: [Organic matter - Refractory](#)

[*RPOM*] – Refractory Particulate Organic Matter

Units	Output Variable Name
mg/L	WQ_RPOM_MG_L
mmol/m ³	WQ_RPOM_MM_M3

Relevant Element: *C*
Atomic Number (Z): 6
Atomic Weight (M): 12
Core Constituent Model: [Organic matter - Refractory](#)

[PHY] - Phytoplankton

Units	Output Variable Name
$\mu\text{g/L}$	WQ_PHYTO_NAME_CONC_MICG_L
mmol/m^3	WQ_PHYTO_NAME_CONC_MM_M3

Relevant Element: *C* (or Chl *a*)

Atomic Number (Z): 6

Atomic Weight (M): 12

Core Constituent Model: [Phytoplankton - Basic](#)

ρ_{PHY} - Cell Density

Output Variable Name: WQ_PHYTO_NAME_DENS_KG_M3

Units: kg/m^3

Core Constituent Model: [Phytoplankton - Basic](#)

[IN] - Internal Nitrogen

Units	Output Variable Name
mg/L	WQ_PHYTO_NAME_INT_N_MG_L
mmol/m^3	WQ_PHYTO_NAME_INT_N_MM_M3

Relevant Element: *N*

Atomic Number (Z): 7

Atomic Weight (M): 14

Core Constituent Model: [Phytoplankton - Advanced](#)

[IP] - Internal Phosphorus

Units	Output Variable Name
mg/L	WQ_PHYTO_NAME_INT_P_MG_L
mmol/m^3	WQ_PHYTO_NAME_INT_P_MM_M3

Relevant Element: *P*

Atomic Number (Z): 15

Atomic Weight (M): 31

Core Constituent Model: [Phytoplankton - Advanced](#)

[SS] - Suspended Sediment

Output Variable Name: SED_N

Units: mg/L

T - Water Temperature

Output Variable Name: TEMP

Units: $^{\circ}\text{C}$

S - Water Salinity

Output Variable Name: SAL**Units:** g/L[NO₂] - Nitrite

Units	Output Variable Name
mg/L	WQ_NITRITE_MG_L
mmol/m ³	WQ_NITRITE_MM_M3

Relevant Element: N**Atomic Number (Z):** 7**Atomic Weight (M):** 14[PTH_a] - Alive Pathogen

Units	Output Variable Name
CFU/100mL	WQ_PATH_NAME_ALIVE_CFU_100ML
check with MEB	WQ_PATH_NAME_ALIVE_CFU_100ML

Core Constituent Model: [Pathogens - Free](#)[PTH_d] - Dead Pathogen

Units	Output Variable Name
CFU/100mL	WQ_PATH_NAME_DEAD_CFU_100ML
check with MEB	WQ_PATH_NAME_DEAD_CFU_100ML

Core Constituent Model: [Pathogens - Free](#)[PTH_t] - Attached Pathogen

Units	Output Variable Name
CFU/100mL	WQ_PATH_NAME_ATTCHD_CFU_100ML
check with MEB	WQ_PATH_NAME_ATTCHD_CFU_100ML

Core Constituent Model: [Pathogens - Attached](#)

P Diagnostic variables

P.1 Overview

The WQ Module's diagnostic output variables, and the core (lowest order) constituent model class and instance where each is deployed are listed below ([Diagnostic Variables](#)).

Each diagnostic variable entry comprises the following components:

- Diagnostic variable heading: The variable symbol in mathematical notation and its full descriptive name.
- Output variable name: Exact string to use in TUFLOW FV output blocks when requesting this variable (see Section [P.1.1](#)). Where both unit systems are supported, variable names and units for both systems are listed in a table. See [Unit Systems](#) for more information on the unit systems.
- Units: The units for the diagnostic variable. Where both unit systems are supported, units are shown as outlined above.
- Science: Where applicable, this links to the equation or science section governing the computation of the diagnostic variable.
- Core Constituent Model: Where applicable, this links to the core constituent model for the diagnostic variable. See Section [2.2.3](#) for details on the available constituent models.
- Description paragraph explaining what the diagnostic variable represents and how to interpret it.

P.1.1 Diagnostic Variable Naming

Below are some key points with regard to naming of diagnostic variables:

- Units are included in the diagnostic variable names, with “ND” signifying “no dimension”.
For example, `WQ_DIAG_PHY_NAME_INT_NUTR_RATIO_ND`
- The text “NAME” in variable names is a placeholder for the user defined phytoplankton group name.
For example, `WQ_DIAG_PHY_NAME_PRIM_PROD_MICG_L_D` would be named `WQ_DIAG_PHY_GREEN_PRIM_PROD_MICG_L_D` if a user defined phytoplankton group name was `Green`
- The text “PHYTO_COM” indicates summed (community level) diagnostics and is not changed by user specification of individual phytoplankton group names
- Output diagnostic variable names are exact, and can therefore be copied and pasted directly into output blocks of control files. The exception is phytoplankton variables, where the user specified group name is included within the variable name, so will need to be inserted by the user.

P.1.2 Interpretation of Diagnostic Variable Outputs

WQ Module calculations are not performed on computational columns of cells that are shallow. In such instances, the reported diagnostic variables are carried from the previous water quality timestep and as such may not reflect actual diagnostics at the reported time. This matter will be addressed in future releases of the WQ Module, however in the interim, caution should be used in the interpretation of diagnostic variables in cells that are known to regularly wet and dry.

In order to preserve shape consistency across all outputs, sheet style diagnostics such as benthic or atmospheric fluxes are reported as fully three dimensional fields. In all cases, these fluxes are reported in the bottom (bed) cell of each computational column (including surface atmospheric fluxes). All other three dimensional cell values are reported as zeros. Therefore, when viewing or interrogating these flux outputs in QGIS, python or MATLAB, the bottom layer of each diagnostic variable should be queried.

In addition, and because diagnostic variables are not tracked or advected and dispersed between timesteps (like computed variables are), they are set to 0 when water quality calculations are turned off in a given cell due to *either* the cell being dry, or it having a water depth less than d_{min-wq} (set via the `Cell Water Quality Depth ==` command). Therefore, care must be taken when interpreting diagnostic variable outputs in cells that are shallower than the specified or default water quality depth.

! Important

The first timestep in all diagnostic variable output files has a value of zero for all cells, because the diagnostic array is initialised at zero before each suite of water quality calculations, including before the first water quality timestep.

As such, when the diagnostic values are written at output file initialisation, all diagnostic values are zero. This contrasts with computed variables written at the same initialisation of output files - these variables are set to the user specified initial conditions. Diagnostic variables do not have corresponding initial conditions and are therefore set to zero on first writing of results.

This should be noted in post processing analyses.

P.2 Diagnostic Variables

$[DO]_{psat}$ - Oxygen Saturation

Output Variable Name: WQ_DIAG_O2_SAT_PCT

Units: %

Science: Equation C.5

Core Constituent Model: Oxygen - O2

Dissolved oxygen percentage saturation that is the equivalent of the dissolved oxygen concentration at current temperature, salinity and pressure conditions

$F_{sed}^{O_2}$ (computed) - Oxygen Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_ACTUAL_O2_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_ACTUAL_O2_SED_FLUX_MMOL_M2_D

Science: Equation C.6

Core Constituent Model: Oxygen - O2

The dynamically computed flux of oxygen across the sediment water interface. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. Multiply by cell area (m²) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be exchanged in that interval

$F_{atm}^{O_2}$ - Oxygen Atmospheric Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_O2_ATMOS_EXCHANGE_MG_M2_D
mmol/m ² /d	WQ_DIAG_O2_ATMOS_EXCHANGE_MMOL_M2_D

Science: Equation C.4

Core Constituent Model: Oxygen - O2

The flux of atmospheric oxygen entering the water column. Positive (negative) values are fluxes to (from) the water column from (to) the atmosphere. Multiply by cell area (m²) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be exchanged in that interval

$F_{sed(computed)}^{Si}$ - Silicate Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_ACTUAL_SI_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_ACTUAL_SI_SED_FLUX_MMOL_M2_D

Science: Equation [D.1](#)

Core Constituent Model: Silicate - Si

The dynamically computed flux of silicate across the sediment water interface. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. Multiply by cell area (m²) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be exchanged in that interval

$F_{sed(computed)}^{NH_4}$ - Ammonium Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_ACTUAL_NH4_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_ACTUAL_NH4_SED_FLUX_MMOL_M2_D

Science: Equation [E.1](#)

Core Constituent Model: Inorganic Nitrogen - AmmoniumNitrate

The dynamically computed flux of ammonium across the sediment water interface. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. Multiply by cell area (m²) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be exchanged in that interval

$F_{sed(computed)}^{NO_3}$ - Nitrate Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_ACTUAL_NO3_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_ACTUAL_NO3_SED_FLUX_MMOL_M2_D

Science: Equation [E.1](#)

Core Constituent Model: Inorganic Nitrogen - AmmoniumNitrate

The dynamically computed flux of nitrate across the sediment water interface. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. Multiply by cell area (m²) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be exchanged in that interval

$F_{nitrif(computed)}^{NH_4}$ - Nitrification Flux

Units	Output Variable Name
mg/L/d	WQ_DIAG_NITRIFICATION_MG_L_D
mmol/m ³ /d	WQ_DIAG_NITRIFICATION_MMOL_M3_D

Science: Equation [E.4](#)

Core Constituent Model: Inorganic Nitrogen - AmmoniumNitrate

The flux of ammonium N to nitrate N due to nitrification. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be exchanged in that interval

$F_{denit(computed)}^{NO_3}$ - Denitrification Flux

Units	Output Variable Name
mg/L/d	WQ_DIAG_DENITRIFICATION_MG_L_D
mmol/m ³ /d	WQ_DIAG_DENITRIFICATION_MMOL_M3_D

Science: Equation [E.7](#)

Core Constituent Model: Inorganic Nitrogen - AmmoniumNitrate

The flux of nitrate N to nitrogen gas N due to denitrification. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be exchanged in that interval

$F_{atm-din(computed)}^N$ - Nitrogen Atmospheric Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_DIN_ATMOS_EXCHANGE_MG_M2_D
mmol/m ² /d	WQ_DIAG_DIN_ATMOS_EXCHANGE_MMOL_M2_D

Science: Equation [E.21](#)

Core Constituent Model: Inorganic Nitrogen - AmmoniumNitrate

The combined wet (rainfall) and dry deposition of inorganic nitrogen across the atmosphere water interface. Positive values are fluxes to the water column from the atmosphere. Multiply by cell area (m²) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be exchanged in that interval

$F_{sed(computed)}^{FRP}$ - FRP Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_ACTUAL_FRP_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_ACTUAL_FRP_SED_FLUX_MMOL_M2_D

Science: Equation [F.1](#)

Core Constituent Model: Inorganic Phosphorus - FRPhs

The dynamically computed flux of FRP across the sediment water interface. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. Multiply by cell area (m²) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be exchanged in that interval

$F_{atm-dip}^{P(computed)}$ - Phosphorus Atmospheric Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_DIP_ATMOS_EXCHANGE_MG_M2_D
mmol/m ² /d	WQ_DIAG_DIP_ATMOS_EXCHANGE_MMOL_M2_D

Science: Equation [F.4](#)

Core Constituent Model: Inorganic Phosphorus - FRPhs

The combined wet (rainfall) and dry deposition of inorganic phosphorus across the atmosphere water interface. Only FRP (FRPads) contributes to wet (dry) deposition. Positive values are fluxes to the water column from the atmosphere. Multiply by cell area (m²) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be exchanged in that interval

$F_{sedmntn}^{POC(computed)}$ - POC Sedimentation Flux

Units	Output Variable Name
mg/L/d	WQ_DIAG_POC_SEDMTN_FLUX_MG_L_D
mmol/m ³ /d	WQ_DIAG_POC_SEDMTN_FLUX_MMOL_M3_D

Science: Equation [M.31](#)

Core Constituent Model: Organic Matter - Labile

The flux of settling labile particulate organic carbon that leaves the water column and enters the sediment. This is not flux of POC from the sediments. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. Multiply by cell volume (L or m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be exchanged in that interval. Although often thought of as being a per area (per m²) loss, the volumetric units of this diagnostic (per L or m³) have been chosen deliberately for consistency with other analogous volumetric losses such as hydrolysis. This is intended to assist in simplifying post processing

$F_{sedmntn}^{PON(computed)}$ - PON Sedimentation Flux

Units	Output Variable Name
mg/L/d	WQ_DIAG_PON_SEDMTN_FLUX_MG_L_D
mmol/m ³ /d	WQ_DIAG_PON_SEDMTN_FLUX_MMOL_M3_D

Science: Equation [M.31](#)

Core Constituent Model: Organic Matter - Labile

The flux of settling labile particulate organic nitrogen that leaves the water column and enters the sediment. This is not flux of PON from the sediments. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. Multiply by cell volume (L or m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be exchanged in that interval. Although often thought of as being a per area (per m²) loss, the volumetric units of this diagnostic (per L or m³) have been chosen deliberately for consistency with other analogous volumetric losses such as hydrolysis. This is intended to assist in simplifying post processing

$F_{sedmntn}^{POP(computed)}$ - POP Sedimentation Flux

Units	Output Variable Name
mg/L/d	WQ_DIAG_POP_SEDMTN_FLUX_MG_L_D
mmol/m ³ /d	WQ_DIAG_POP_SEDMTN_FLUX_MMOL_M3_D

Science: Equation [M.31](#)

Core Constituent Model: Organic Matter - Labile

The flux of settling labile particulate organic phosphorus that leaves the water column and enters the sediment. This is not flux of POP from the sediments. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. Multiply by cell volume (L or m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be exchanged in that interval. Although often thought of as being a per area (per m²) loss, the volumetric units of this diagnostic (per L or m³) have been chosen deliberately for consistency with other analogous volumetric losses such as hydrolysis. This is intended to assist in simplifying post processing

$CDOM_{(computed)}$ - CDOM

Output Variable Name: WQ_DIAG_CHRMPHC DISS_ORGS_M

Units: /m

Science: Equation [M.22](#)

Core Constituent Model: Organic Matter - Refractory

Chromophoric dissolved organic matter. It is the equivalent extinction coefficient for absorption of radiation at 440 nm. It is computed from DOC (and RDOC if refractory organic matter is simulated) and uses the relationship of Equation [M.22](#)

$F_{sed(computed)}^{DOC}$ - DOC Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_ACTUAL_DOC_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_ACTUAL_DOC_SED_FLUX_MMOL_M2_D

Science: Equation [M.1](#)

Core Constituent Model: Organic Matter - Labile

The dynamically computed flux of DOC across the sediment water interface. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. Multiply by cell area (m²) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be exchanged in that interval

$F_{sed(computed)}^{DON}$ - DON Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_ACTUAL_DON_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_ACTUAL_DON_SED_FLUX_MMOL_M2_D

Science: Equation [M.1](#)

Core Constituent Model: Organic Matter - Labile

The dynamically computed flux of DON across the sediment water interface. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. Multiply by cell area (m²) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be exchanged in that interval

$F_{sed(computed)}^{DOP}$ - DOP Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_ACTUAL_DOP_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_ACTUAL_DOP_SED_FLUX_MMOL_M2_D

Science: Equation [M.1](#)

Core Constituent Model: Organic Matter - Labile

The dynamically computed flux of DOP across the sediment water interface. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. Multiply by cell area (m²) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be exchanged in that interval

$F_{hyd(computed)}^{POC}$ - POC Hydrolysis Flux

Units	Output Variable Name
mg/L/d	WQ_DIAG_POC_HYDROL_MG_L_D
mmol/m ³ /d	WQ_DIAG_POC_HYDROL_MMOL_M3_D

Science: Equation [M.3](#)

Core Constituent Model: Organic Matter - Labile

The flux of labile POC to labile DOC due to hydrolysis. Values are only positive. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be hydrolysed in that interval

$F_{miner(computed)}^{DOC}$ - DOC Mineralisation Flux

Units	Output Variable Name
mg/L/d	WQ_DIAG_DOC_MINERL_MG_L_D
mmol/m ³ /d	WQ_DIAG_DOC_MINERL_MMOL_M3_D

Science: Equation [M.9](#)

Core Constituent Model: Organic Matter - Labile

The flux of labile DOC to DIC due to mineralisation. Values are only positive. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be mineralised in that interval

$F_{hyd(computed)}^{PON}$ - PON Hydrolysis Flux

Units	Output Variable Name
mg/L/d	WQ_DIAG_PON_HYDROL_MG_L_D
mmol/m ³ /d	WQ_DIAG_PON_HYDROL_MMOL_M3_D

Science: Equation [M.3](#)

Core Constituent Model: Organic Matter - Labile

The flux of labile PON to labile DON due to hydrolysis. Values are only positive. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be hydrolysed in that interval

$F_{miner(computed)}^{DON}$ - DON Mineralisation Flux

Units	Output Variable Name
mg/L/d	WQ_DIAG_DON_MINERL_MG_L_D
mmol/m ³ /d	WQ_DIAG_DON_MINERL_MMOL_M3_D

Science: Equation [M.9](#)

Core Constituent Model: Organic Matter - Labile

The flux of labile DON to ammonium due to mineralisation. Values are only positive. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be mineralised in that interval

$F_{hyd(computed)}^{POP}$ - POP Hydrolysis Flux

Units	Output Variable Name
mg/L/d	WQ_DIAG_POP_HYDROL_MG_L_D
mmol/m ³ /d	WQ_DIAG_POP_HYDROL_MMOL_M3_D

Science: Equation [M.3](#)

Core Constituent Model: Organic Matter - Labile

The flux of labile POP to labile DOP due to hydrolysis. Values are only positive. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be hydrolysed in that interval

$F_{miner(computed)}^{DOP}$ - DOP Mineralisation Flux

Units	Output Variable Name
mg/L/d	WQ_DIAG_DOP_MINERL_MG_L_D
mmol/m ³ /d	WQ_DIAG_DOP_MINERL_MMOL_M3_D

Science: Equation [M.9](#)

Core Constituent Model: Organic Matter - Labile

The flux of labile DOP to FRP due to mineralisation. Values are only positive. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be mineralised in that interval

$F_{miner(computed)}^{an}$ - DOC Anaerobic Mineralisation Flux

Units	Output Variable Name
mg/L/d	WQ_DIAG_DOC_MINERL_AN_MG_L_D
mmol/m ³ /d	WQ_DIAG_DOC_MINERL_AN_MMOL_M3_D

Science: Equation [M.15](#)

Core Constituent Model: Organic Matter - Labile

The component of the mineralisation flux of labile dissolved organic carbon that is anaerobic, i.e. the mineralisation that occurs after oxygen has been consumed from both diatomic dissolved oxygen and nitrate. Multiply by cell volume (m^3) and time interval of interest (seconds / 86400) to compute the mass (or moles) of carbon that would be anaerobically mineralised in that interval. Reporting units of this diagnostic are carbon

$F_{miner}^{NO_3}(\text{computed})$ - DOC Denitification Mineralisation

Units	Output Variable Name
mg/L/d	WQ_DIAG_DOC_MINERL_DENIT_MG_L_D
mmol/ m^3 /d	WQ_DIAG_DOC_MINERL_DENIT_MMOL_M3_D

Science: Equation [M.14](#)

Core Constituent Model: Organic Matter - Labile

The component of the mineralisation flux of labile dissolved organic carbon that occurs following consumption of dissolved oxygen, and that sources its oxygen from stripping (denitrifying) nitrate. It is the mineralisation that occurs after oxygen has been consumed from diatomic dissolved oxygen but before anaerobic mineralisation occurs. Multiply by cell volume (m^3) and time interval of interest (seconds / 86400) to compute the mass (or moles) of carbon that would be aerobically mineralised in that interval. The same number of moles of nitrate N will be consumed. Reporting units of this diagnostic are carbon

$BOD5^{O_2}(\text{computed})$ - BOD5

Output Variable Name: WQ_DIAG_DOC_BOD5_MG_L

Units: mg/L

Science: Equation [M.13](#)

Core Constituent Model: Organic Matter - Labile

The reduction in the concentration of dissolved oxygen that would result by the action of aerobic mineralisation of dissolved organic carbon over a period of 5 days. It is computed at the instantaneous oxygen consumption rate

$V_{settle}^{lorg}(\text{computed})$ - Labile Particulate Organic Matter Settling Velocity

Output Variable Name: WQ_DIAG_POM_VERT_VEL_M_S

Units: m/s

Science: Section [M.8](#)

Core Constituent Model: Organic Matter - Labile

The computed settling velocity of labile particulate organic carbon, nitrogen and phosphorus (which all have the same velocity). Positive (negative) values are upwards (downwards)

$F_{sedmtn}^{RPOM}(\text{computed})$ - RPOM Sedimentation Flux

Units	Output Variable Name
mg/L/d	WQ_DIAG_RPOM_SEDMTN_FLUX_MG_L_D
mmol/ m^3 /d	WQ_DIAG_RPOM_SEDMTN_FLUX_MMOL_M3_D

Science: Equation [M.32](#)

Core Constituent Model: Organic Matter - Refractory

The flux of settling refractory particulate organic matter that leaves the water column and enters the sediment. This is not flux of RPOM from the sediments. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. Multiply by cell volume (L or m^3) and time interval of interest (seconds / 86400) to compute the

mass (or moles) that would be exchanged in that interval. Although often thought of as being a per area (per m²) loss, the volumetric units of this diagnostic (per L or m³) have been chosen deliberately for consistency with other analogous volumetric losses such as photolysis. This is intended to assist in simplifying post processing

$F_{photo(computed)}^{RDOC}$ - RPOM Photolysis

Units	Output Variable Name
mg/L/d	WQ_DIAG_PHOTOLYSIS_MG_L_D
mmol/m ³ /d	WQ_DIAG_PHOTOLYSIS_MMOL_M3_D

Science: Equation [M.23](#)

Core Constituent Model: Organic Matter - Refractory

The flux of refractory dissolved organic carbon to labile dissolved organic carbon and potentially DIC (if f_{photo}^{DOM} is not 1.0). This flux is always positive and is the carbon fraction only. Equivalent nitrogen and phosphorus fraction fluxes can be computed as per Equation [M.23](#)

$V_{settle(computed)}^{rorg}$ - Refractory Particulate Organic Matter Settling Velocity

Output Variable Name: WQ_DIAG_RPOM_VERT_VEL_M_S

Units: m/s

Science: Section [M.8](#)

Core Constituent Model: Organic Matter - Refractory

The computed settling velocity of refractory particulate organic matter. Positive (negative) values are upwards (downwards)

R_{IN-IP}^{phy} - Ratio of Internal Nutrients

Output Variable Name: WQ_DIAG_PHY_NAME_INT_NUTR_RATIO_ND

Units: dimensionless

Core Constituent Model: Phytoplankton - Basic

The ratio of internal nitrogen to internal phosphorus for a phytoplankton group. This quantity is reported for both the basic and advanced phytoplankton constituent models, with the former being the constant quotient of user (or default) internal nitrogen and phosphorus to carbon ratios. If the latter, this diagnostic will vary between the quotients of the user defined (or default) minimum and maximum limits of internal nitrogen and phosphorus to carbon ratios. Although noted here as being dimensionless, this quantity can be thought of as having units of (N concentration) / (P concentration)

I_{light}^{phy} - Light Limitation Function

Output Variable Name: WQ_DIAG_PHY_NAME_LGHT_LIM_ND

Units: 0

Science: Section [I.6](#)

Core Constituent Model: Phytoplankton - Basic

The dynamically computed light limitation function for a phytoplankton group. It varies between 0 (complete limitation) and 1 (no limitation)

I_{nit}^{phy} - Nitrogen Limitation Function

Output Variable Name: WQ_DIAG_PHY_NAME_N_LIM_ND

Units: dimensionless

Science: Section [I.3](#)

Core Constituent Model: Phytoplankton - Basic

The dynamically computed nitrogen limitation function for a phytoplankton group. It varies between 0 (complete limitation) and 1 (no limitation)

L_{phy}^{phs} - Phosphorus Limitation Function

Output Variable Name: WQ_DIAG_PHY_NAME_P_LIM_ND

Units: dimensionless

Science: Section [I.4](#)

Core Constituent Model: Phytoplankton - Basic

The dynamically computed phosphorus limitation function for a phytoplankton group. It varies between 0 (complete limitation) and 1 (no limitation)

L_{phy}^{sil} - Silicate Limitation Function

Output Variable Name: WQ_DIAG_PHY_NAME_SI_LIM_ND

Units: dimensionless

Science: Section [I.5](#)

Core Constituent Model: Phytoplankton - Basic

The dynamically computed silicate limitation function for a phytoplankton group. It varies between 0 (complete limitation) and 1 (no limitation)

L_T^{phy} - Temperature Limitation Function

Output Variable Name: WQ_DIAG_PHY_NAME_TMPTR_LIM_ND

Units: dimensionless

Science: Section [I.2](#)

Core Constituent Model: Phytoplankton - Basic

The dynamically computed temperature limitation function for a phytoplankton group. It varies between 0 (complete limitation) and a positive number. This limitation function value can be greater than 1, and in such instances this represents an opportunity for augmented phytoplankton growth (subject to the values of other related limitation functions)

L_{sal-r}^{phy} - Salinity Limitation Function

Output Variable Name: WQ_DIAG_PHY_NAME_SAL_LIM_ND

Units: dimensionless

Science: Section [I.7](#)

Core Constituent Model: Phytoplankton - Basic

The dynamically computed salinity limitation function applied to respiration of a phytoplankton group. It is always greater than 1 (no limitation). The same diagnostic variable name is used for the corollary primary productivity salinity limitation function because the two limitation functions are mutually exclusive

L_{sal-pp}^{phy} - Salinity Limitation Function

Output Variable Name: WQ_DIAG_PHY_NAME_SAL_LIM_ND

Units: dimensionless

Science: Section [I.7](#)

Core Constituent Model: Phytoplankton - Basic

The dynamically computed salinity limitation function applied to primary production of a phytoplankton group. It varies between 0 (complete limitation) and 1 (no limitation). The same diagnostic variable name is used for the corollary respiration salinity limitation function because the two limitation functions are mutually exclusive

$F_{prod(computed)}^{phy}$ - Phytoplankton Primary Productivity

Units	Output Variable Name
$\mu\text{g/L/d}$	WQ_DIAG_PHY_NAME_PRIM_PROD_MICG_L_D
$\text{mmol/m}^3/\text{d}$	WQ_DIAG_PHY_NAME_PRIM_PROD_MMOL_M3_D

Science: Equation [H.5](#)

Core Constituent Model: Phytoplankton - Basic

The flux of carbon to phytoplankton as a result of productivity, without accounting for respiration, for a phytoplankton group. Also referred to as growth or gross primary productivity, and typically associated with daytime phytoplankton photosynthesis. Values are only positive. Multiply by cell volume (m^3) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be taken up via productivity in that interval

$F_{sedmntn(computed)}^{phy}$ - Phytoplankton Sedimentation

Units	Output Variable Name
$\mu\text{g/L/d}$	WQ_DIAG_PHY_NAME_SEDMNTN_MICG_L_D
$\text{mmol/m}^3/\text{d}$	WQ_DIAG_PHY_NAME_SEDMNTN_MMOL_M3_D

Science: Equation [H.13](#)

Core Constituent Model: Phytoplankton - Basic

The flux of phytoplankton chlorophyll *a* (or carbon) into the sediments as a result of settling for a phytoplankton group. Values are only losses and are only negative. Multiply by cell volume (L or m^3) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be lost to settling in that interval. Although often thought of as being a per area (per m^2) loss, the volumetric units of this diagnostic (per L or m^3) have been chosen deliberately for consistency with other analogous volumetric losses such as mortality. This is intended to assist in simplifying post processing

V_{settle}^{phy} - Phytoplankton Settling velocity

Output Variable Name: WQ_DIAG_PHY_NAME_VERT_VEL_M_S

Units: m/s

Science: Section [H.4](#)

Core Constituent Model: Phytoplankton - Basic

Phytoplankton settling velocity, as computed from the user specified (or default) method, for a phytoplankton group. Upwards (downwards) is negative (positive)

$F_{sedmntn(computed)}^{comm}$ - Community Phytoplankton Sedimentation

Units	Output Variable Name
$\mu\text{g/L/d}$	WQ_DIAG_PHYTO_COM_SEDMNTN_MICG_L_D
$\text{mmol/m}^3/\text{d}$	WQ_DIAG_PHYTO_COM_SEDMNTN_MMOL_M3_D

Science: Equation [H.13](#)

Core Constituent Model: Phytoplankton - Basic

The flux of phytoplankton into the sediments as a result of settling, summed over all phytoplankton groups (i.e. a simulation's phytoplankton community). Values are only losses and are only negative. Multiply by cell volume

(L or m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be lost to settling in that interval. Although often thought of as being a per area (per m²) loss, the volumetric units of this diagnostic (per L or m³) have been chosen deliberately for consistency with other analogous losses such as individual phytoplankton group sedimentation rates. This is intended to assist in simplifying post processing

$F_{prod(computed)}^{comm}$ - Community Primary Productivity

Units	Output Variable Name
μg/L/d	WQ_DIAG_PHYTO_COM_PRIM_PROD_MICG_L_D
mmol/m ³ /d	WQ_DIAG_PHYTO_COM_PRIM_PROD_MMOL_M3_D

Science: Equation [H.5](#)

Core Constituent Model: Phytoplankton - Basic

The flux of carbon (and nutrients) to phytoplankton as a result of productivity, without accounting for respiration, summed over all phytoplankton groups (i.e. a simulation's phytoplankton community). Also referred to as growth, and typically associated with daytime phytoplankton photosynthesis. Values are only positive. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be taken up via productivity in that interval

$F_{netprod(computed)}^{comm}$ - Community Net Primary Productivity

Units	Output Variable Name
μg/L/d	WQ_DIAG_PHYTO_COM_NET_PROD_MICG_L_D
mmol/m ³ /d	WQ_DIAG_PHYTO_COM_NET_PROD_MMOL_M3_D

Science: Equation [H.9](#)

Core Constituent Model: Phytoplankton - Basic

The flux of carbon (and nutrients) to phytoplankton as a result of productivity, accounting for respiration losses due only to the consumption of stored energy, summed over all phytoplankton groups (i.e. a simulation's phytoplankton community). Also referred to as net primary productivity. Values are only positive. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be taken up via net productivity in that interval

$R_{PP-resp}^{comm}$ - Community Primary Productivity Ratio

Output Variable Name: WQ_DIAG_PHYTO_COM_PROD_RESP_R_

Units: dimensionless

Ratio of primary productivity to true respiration, summed over all phytoplankton groups (i.e. a simulation's phytoplankton community). **Currently inactive and reported as 999**

$R_{NPP-resp}^{comm}$ - Community Net Primary Productivity Ratio

Output Variable Name: WQ_DIAG_PHYTO_COM_NET_RESP_R_

Units: dimensionless

Ratio of net primary productivity to true respiration, summed over all phytoplankton groups (i.e. a simulation's phytoplankton community). **Currently inactive and reported as 999**

$F_{nit-uptake}^{comm}$ (computed) - Community Nitrate Uptake

Units	Output Variable Name
mg/L/d	WQ_DIAG_PHYTO_COM_NO3_UPTAKE_MG_L_D
mmol/m ³ /d	WQ_DIAG_PHYTO_COM_NO3_UPTAKE_MMOL_M3_D

Science: Equation J.3

Core Constituent Model: Phytoplankton - Basic

The flux of nitrate to phytoplankton as a result of productivity, summed over all phytoplankton groups (i.e. a simulation's phytoplankton community). Values are only positive. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be taken up in that interval. Although computed differently for the basic and advanced phytoplankton constituent models, the interpretation of this quantity is the same for both

$F_{amm-uptake}^{comm}$ (computed) - Community Ammonium Uptake

Units	Output Variable Name
mg/L/d	WQ_DIAG_PHYTO_COM_NH4_UPTAKE_MG_L_D
mmol/m ³ /d	WQ_DIAG_PHYTO_COM_NH4_UPTAKE_MMOL_M3_D

Science: Equation J.3

Core Constituent Model: Phytoplankton - Basic

The flux of ammonium to phytoplankton as a result of productivity, summed over all phytoplankton groups (i.e. a simulation's phytoplankton community). Values are only positive. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be taken up in that interval. Although computed differently for the basic and advanced phytoplankton constituent models, the interpretation of this quantity is the same for both

$F_{P-uptake}^{comm}$ (computed) - Community FRP Uptake

Units	Output Variable Name
mg/L/d	WQ_DIAG_PHYTO_COM_P_UPTAKE_MG_L_D
mmol/m ³ /d	WQ_DIAG_PHYTO_COM_P_UPTAKE_MMOL_M3_D

Science: Equation J.7

Core Constituent Model: Phytoplankton - Basic

The flux of FRP to phytoplankton as a result of productivity, summed over all phytoplankton groups (i.e. a simulation's phytoplankton community). Values are only positive. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be taken up in that interval. Although computed differently for the basic and advanced phytoplankton constituent models, the interpretation of this quantity is the same for both

$F_{C-uptake}^{comm}$ (computed) - Community Carbon Uptake

Units	Output Variable Name
$\mu\text{g/L/d}$	WQ_DIAG_PHYTO_COM_C_UPTAKE_MG_L_D
$\text{mmol/m}^3/\text{d}$	WQ_DIAG_PHYTO_COM_C_UPTAKE_MMOL_M3_D

Science: Equation [J.1](#)

Core Constituent Model: Phytoplankton - Basic

The flux of carbon (and nutrients) to phytoplankton as a result of productivity, without accounting for respiration, summed over all phytoplankton groups (i.e. a simulation's phytoplankton community). Also referred to as growth, and typically associated with daytime phytoplankton photosynthesis. Values are only positive. Multiply by cell volume (m^3) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be taken up via productivity in that interval. This is numerically the same as primary productivity

PAR - Community PAR

Output Variable Name: WQ_DIAG_PHYTO_COM_PAR_W_M2

Units: W/m^2

Science: Section [2.3.2](#)

Core Constituent Model: Phytoplankton - Basic

The ambient PAR field in each computational cell, as set by the hydrodynamic model

$[\text{Chla}]^{\text{comm}}$ - Community chlorophyll a

Output Variable Name: WQ_DIAG_PHYTO_COM_TCHLA_MICG_L

Units: $\mu\text{g/L}$

Core Constituent Model: Phytoplankton - Basic

The total chlorophyll a summed across all phytoplankton groups

$[\text{Chla}]^{\text{comm}}$ - Community Phytoplankton Concentration

Units	Output Variable Name
mmol/m^3	WQ_DIAG_PHYTO_COM_TPHY_MMOL_C_M3
mmol/m^3	WQ_DIAG_PHYTO_COM_TPHY_MMOL_C_M3

Core Constituent Model: Phytoplankton - Basic

The concentration of phytoplankton in mmols of carbon, summed over all phytoplankton groups (i.e. a simulation's phytoplankton community). Multiplying this number by 12 and dividing (on a cell by cell basis) by the equivalent Community chlorophyll a value (as reported, i.e. in $\mu\text{g/L}$) will result in an array of the average carbon to chlorophyll a ratio of the community for each cell. This is effectively a concentration weighted average of the individual phytoplankton group carbon to chlorophyll a ratios at any given time and in any given cell

$[\text{N}]_{\text{in}}^{\text{comm}}$ - Community Internal Nitrogen Concentration

Units	Output Variable Name
$\mu\text{g/L}$	WQ_DIAG_PHYTO_COM_T_IN_N_MG_L
mmol/m^3	WQ_DIAG_PHYTO_COM_T_IN_N_MMOL_M3

Science: Section J.2.2

Core Constituent Model: Phytoplankton - Basic

The internal nitrogen concentration of phytoplankton, summed over all phytoplankton groups (i.e. a simulation's phytoplankton community), for both the basic and advanced phytoplankton constituent models

$[P]_{in}^{comm}$ - Community Internal Phosphorus Concentration

Units	Output Variable Name
$\mu\text{g/L}$	WQ_DIAG_PHYTO_COM_T_IN_P_MG_L
mmol/m^3	WQ_DIAG_PHYTO_COM_T_IN_P_MMOL_M3

Science: Section J.3.2

Core Constituent Model: Phytoplankton - Basic

The internal phosphorus concentration of phytoplankton, summed over all phytoplankton groups (i.e. a simulation's phytoplankton community), for both the basic and advanced phytoplankton constituent models

$F_{sed}^{O_2}$ - Oxygen User Defined Sediment Flux

Units	Output Variable Name
$\text{mg/m}^2/\text{d}$	WQ_DIAG_INPUT_O2_SED_FLUX_MG_M2_D
$\text{mmol/m}^2/\text{d}$	WQ_DIAG_INPUT_O2_SED_FLUX_MMOL_M2_D

Science: Equation C.6

Core Constituent Model: Oxygen - O₂

The user defined (or model default) flux of oxygen across the sediment water interface. This value is reported for completeness and should not change in time for a given cell. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. This diagnostic cannot be used in mass balance or other related calculations

F_{sed}^{Si} - Silicate User Defined Sediment Flux

Units	Output Variable Name
$\text{mg/m}^2/\text{d}$	WQ_DIAG_INPUT_SI_SED_FLUX_MG_M2_D
$\text{mmol/m}^2/\text{d}$	WQ_DIAG_INPUT_SI_SED_FLUX_MMOL_M2_D

Science: Equation D.1

Core Constituent Model: Silicate - Si

The user defined (or model default) flux of silicate across the sediment water interface. This value is reported for completeness and should not change in time for a given cell. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. This diagnostic cannot be used in mass balance or other related calculations

$F_{sed}^{NH_4}$ - Ammonium User Defined Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_INPUT_NH4_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_INPUT_NH4_SED_FLUX_MMOL_M2_D

Science: Equation [E.1](#)

Core Constituent Model: Inorganic Nitrogen - AmmoniumNitrate

The user defined (or model default) flux of ammonium across the sediment water interface. This value is reported for completeness and should not change in time for a given cell. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. This diagnostic cannot be used in mass balance or other related calculations

$F_{sed}^{NO_3}$ - Nitrate User Defined Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_INPUT_NO3_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_INPUT_NO3_SED_FLUX_MMOL_M2_D

Science: Equation [E.1](#)

Core Constituent Model: Inorganic Nitrogen - AmmoniumNitrate

The user defined (or model default) flux of nitrate across the sediment water interface. This value is reported for completeness and should not change in time for a given cell. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. This diagnostic cannot be used in mass balance or other related calculations

F_{sed}^{FRP} - FRP User Defined Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_INPUT_FRP_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_INPUT_FRP_SED_FLUX_MMOL_M2_D

Science: Equation [F.1](#)

Core Constituent Model: Inorganic Phosphorus - FRPhs

The user defined (or model default) flux of FRP across the sediment water interface. This value is reported for completeness and should not change in time for a given cell. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. This diagnostic cannot be used in mass balance or other related calculations

F_{sed}^{DOC} - DOC User Defined Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_INPUT_DOC_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_INPUT_DOC_SED_FLUX_MMOL_M2_D

Science: Equation [M.1](#)

Core Constituent Model: Organic Matter - Labile

The user defined (or model default) flux of DOC across the sediment water interface. This value is reported for completeness and should not change in time for a given cell. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. This diagnostic cannot be used in mass balance or other related calculations

F_{sed}^{DON} – DON User Defined Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_INPUT_DON_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_INPUT_DON_SED_FLUX_MMOL_M2_D

Science: Equation [M.1](#)

Core Constituent Model: Organic Matter - Labile

The user defined (or model default) flux of DON across the sediment water interface. This value is reported for completeness and should not change in time for a given cell. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. This diagnostic cannot be used in mass balance or other related calculations

F_{sed}^{DOP} – DOP User Defined Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_INPUT_DOP_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_INPUT_DOP_SED_FLUX_MMOL_M2_D

Science: Equation [M.1](#)

Core Constituent Model: Organic Matter - Labile

The user defined (or model default) flux of DOP across the sediment water interface. This value is reported for completeness and should not change in time for a given cell. Positive (negative) values are fluxes to (from) the water column from (to) the sediment. This diagnostic cannot be used in mass balance or other related calculations

TN – Total Nitrogen

Units	Output Variable Name
mg/L	WQ_DIAG_TOTAL_NITROGEN_MG_L
mmol/m ³	WQ_DIAG_TOTAL_NITROGEN_MMOL_M3

The sum of relevant nitrogen species. These are:

- Simulation class DO: None
- Simulation class Inorganics: ammonium, nitrate, phytoplankton internal nitrogen (whether it is a simulated variable or not it still contributes to total nitrogen)
- Simulation class Organics: ammonium, nitrate, phytoplankton internal nitrogen, DON, PON and RDON if refractory organic constituent model is used

TP – Total Phosphorus

Units	Output Variable Name
mg/L	WQ_DIAG_TOTAL_PHOSPHORUS_MG_L
mmol/m ³	WQ_DIAG_TOTAL_PHOSPHORUS_MMOL_M3

The sum of relevant phosphorus species. These are:

- Simulation class DO: None
- Simulation class Inorganics: FRP, adsorbed FRP if simulated, phytoplankton internal phosphorus (whether it is a simulated variable or not it still contributes to total phosphorus)
- Simulation class Organics: FRP, adsorbed FRP if simulated, phytoplankton internal phosphorus, DOP, POP and RDOP if refractory organic constituent model is used

TKN - Total Kjeldahl Nitrogen

Units	Output Variable Name
mg/L	WQ_DIAG_TOTAL_KJELDAHL_NITROGEN_MG_L
mmol/m ³	WQ_DIAG_TOTAL_KJELDAHL_NITROGEN_MMOL_M3

The sum of relevant nitrogen species. These are:

- Simulation class DO: None
- Simulation class Inorganics: ammonium, phytoplankton internal nitrogen (whether it is a simulated variable or not it still contributes to total nitrogen)
- Simulation class Organics: ammonium, phytoplankton internal nitrogen, DON, PON and RDON if refractory organic constituent model is used

TOC - Total organic carbon

Units	Output Variable Name
mg/L	WQ_DIAG_TOTAL_ORGANIC_CARBON_MG_L
mmol/m ³	WQ_DIAG_TOTAL_ORGANIC_CARBON_MMOL_M3

The sum of relevant carbon species. These are:

- Simulation class DO: None
- Simulation class Inorganics: phytoplankton carbon
- Simulation class Organics: phytoplankton carbon, DOC, POC, and RDOC and RPOM if refractory organic constituent model is used

F_{sed}^{POC} - POC User Defined Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_INPUT_POC_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_INPUT_POC_SED_FLUX_MMOL_M2_D

Currently unused and reported as zero. Will be activated in future releases

F_{sed}^{PON} - PON User Defined Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_INPUT_PON_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_INPUT_PON_SED_FLUX_MMOL_M2_D

Currently unused and reported as zero. Will be activated in future releases

F_{sed}^{POP} - POP User Defined Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_INPUT_POP_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_INPUT_POP_SED_FLUX_MMOL_M2_D

Currently unused and reported as zero. Will be activated in future releases

$F_{sed(computed)}^{POC}$ - POC Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_ACTUAL_POC_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_ACTUAL_POC_SED_FLUX_MMOL_M2_D

Currently unused and reported as the same as WQ_DIAG_POC_SEDMTN_FLUX_MG_M2_D. Will be activated in future releases

$F_{sed(computed)}^{PON}$ - PON Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_ACTUAL_PON_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_ACTUAL_PON_SED_FLUX_MMOL_M2_D

Currently unused and reported as the same as WQ_DIAG_PON_SEDMTN_FLUX_MG_M2_D. Will be activated in future releases

$F_{sed(computed)}^{POP}$ - POP Sediment Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_ACTUAL_POP_SED_FLUX_MG_M2_D
mmol/m ² /d	WQ_DIAG_ACTUAL_POP_SED_FLUX_MMOL_M2_D

Currently unused and reported as the same as WQ_DIAG_POP_SEDMTN_FLUX_MG_M2_D. Will be activated in future releases

M_{sed}^{OC} - Organic Carbon Sediment Mass

Units	Output Variable Name
mg/m ²	WQ_DIAG_SEDIMENT_ORGC_MASS_MG_M2
mmol/m ²	WQ_DIAG_SEDIMENT_ORGC_MASS_MMOL_M2

Currently unused and reported as zero. Will be activated in future releases

M_{sed}^{ON} - Organic Nitrogen Sediment Mass

Units	Output Variable Name
mg/m ²	WQ_DIAG_SEDIMENT_ORGN_MASS_MG_M2
mmol/m ²	WQ_DIAG_SEDIMENT_ORGN_MASS_MMOL_M2

Currently unused and reported as zero. Will be activated in future releases

M_{sed}^{OP} - Organic Phosphorus Sediment Mass

Units	Output Variable Name
mg/m ²	WQ_DIAG_SEDIMENT_ORGP_MASS_MG_M2
mmol/m ²	WQ_DIAG_SEDIMENT_ORGP_MASS_MMOL_M2

Currently unused and reported as zero. Will be activated in future releases

F_{resus}^{POC} - POC Resuspension Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_POC_RESUS_MG_M2_D
mmol/m ² /d	WQ_DIAG_POC_RESUS_MMOL_M2_D

Currently unused and reported as zero. Will be activated in future releases

F_{resus}^{PON} - PON Resuspension Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_PON_RESUS_MG_M2_D
mmol/m ² /d	WQ_DIAG_PON_RESUS_MMOL_M2_D

Currently unused and reported as zero. Will be activated in future releases

F_{resus}^{POP} - POP Resuspension Flux

Units	Output Variable Name
mg/m ² /d	WQ_DIAG_POP_RESUS_MG_M2_D
mmol/m ² /d	WQ_DIAG_POP_RESUS_MMOL_M2_D

Currently unused and reported as zero. Will be activated in future releases

F_{N-fix}^{comm} - Community Nitrogen Fixing Uptake

Units	Output Variable Name
mg/L/d	WQ_DIAG_PHYTO_COM_N2_UPTAKE_MG_L_D
mmol/m ³ /d	WQ_DIAG_PHYTO_COM_N2_UPTAKE_MMOL_M3_D

The flux of atmospheric nitrogen fixed by phytoplankton, summed over all phytoplankton groups (i.e. a simulation's phytoplankton community), for both the basic and advanced phytoplankton constituent models

$F_{anmx(computed)}^{N_2}$ - Anaerobic Oxidation of Ammonium

Units	Output Variable Name
mg/L/d	WQ_DIAG_ANAER_NH4_OX_MG_L_D
mmol/m ³ /d	WQ_DIAG_ANAER_NH4_OX_MMOL_M3_D

Science: Equation [E.10](#)

Core Constituent Model: Inorganic Nitrogen - AmmoniumNitrate

The flux of ammonium-N and nitrate-N to free diatomic nitrogen gas (also referred to as anammox). Values are only positive. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) on N that would be lost via anammox in that interval. The diagnostic variable is the production of nitrogen gas N (not N₂)

$F_{DRNA}^{NO_3}$ (computed) - Dissimilatory Reduction of Nitrate to Ammonium

Units	Output Variable Name
mg/L/d	WQ_DIAG DISS_NO3_RED_MG_L_D
mmol/m ³ /d	WQ_DIAG DISS_NO3_RED_MMOL_M3_D

Science: Equation [E.12](#)

Core Constituent Model: Inorganic Nitrogen - AmmoniumNitrate

The flux of nitrate-N to ammonium-N (also referred to as DRNA). Values are only positive. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) on N that would be lost via DRNA in that interval

F_{bdn}^{RPOM} (computed) - RPOM Breakdown

Units	Output Variable Name
mg/L/d	WQ_DIAG_RPOM_BREAKDOWN_MG_L_D
mmol/m ³ /d	WQ_DIAG_RPOM_BREAKDOWN_MMOL_M3_D

Science: Equation [M.6](#)

Core Constituent Model: Organic Matter - Refractory

The flux of refractory particulate organic matter to labile particulate organic matter under microbial activity. This flux is always positive and is applied directly to the carbon fraction of RPOM. Equivalent nitrogen and phosphorus fraction fluxes are computed proportionately as per Equation [M.7](#)

F_{act}^{RDOC} (computed) - RDOC Activation

Units	Output Variable Name
mg/L/d	WQ_DIAG_RDOC_ACTV_MG_L_D
mmol/m ³ /d	WQ_DIAG_RDOC_ACTV_MMOL_M3_D

Science: Equation [M.18](#)

Core Constituent Model: Organic Matter - Refractory

The flux of refractory dissolved organic carbon to labile dissolved organic carbon under microbial activity. This flux is always positive

F_{act}^{RDON} (computed) - RDON Activation

Units	Output Variable Name
mg/L/d	WQ_DIAG_RDON_ACTV_MG_L_D
mmol/m ³ /d	WQ_DIAG_RDON_ACTV_MMOL_M3_D

Science: Equation [M.18](#)

Core Constituent Model: Organic Matter - Refractory

The flux of refractory dissolved organic nitrogen to labile dissolved organic nitrogen under microbial activity. This flux is always positive

$F_{act(computed)}^{RDOP}$ - RDOP Activation

Units	Output Variable Name
mg/L/d	WQ_DIAG_RDOP_ACTV_MG_L_D
mmol/m ³ /d	WQ_DIAG_RDOP_ACTV_MMOL_M3_D

Science: Equation [M.18](#)

Core Constituent Model: Organic Matter - Refractory

The flux of refractory dissolved organic phosphorus to labile dissolved organic phosphorus under microbial activity. This flux is always positive

$F_{resp(computed)}^{phy}$ - Phytoplankton Respiration

Units	Output Variable Name
μg/L/d	WQ_DIAG_PHY_NAME_RESP_MICG_L_D
mmol/m ³ /d	WQ_DIAG_PHY_NAME_RESP_MMOL_M3_D

Science: Equation [H.8](#)

Core Constituent Model: Phytoplankton - Basic

The flux of carbon from phytoplankton as a result of energy consumption (referred to as true respiration). It is typically seen as a night time phytoplanktonic process but can also occur during the day. Values are only negative. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be lost via true respiration in that interval

$F_{resp-N(computed)}^{phy}$ - Phytoplankton Respiration - Nitrogen

Units	Output Variable Name
mg/L/d	WQ_DIAG_PHY_NAME_RESP_N_MG_L_D
mmol/m ³ /d	WQ_DIAG_PHY_NAME_RESP_N_MMOL_M3_D

Science: Equation [H.10](#)

Core Constituent Model: Phytoplankton - Basic

The flux of nitrogen from phytoplankton as a result of energy consumption (referred to as true respiration). It is typically seen as a night time phytoplanktonic process but can also occur during the day. Values are only negative. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be lost via true respiration in that interval

$F_{resp-P(computed)}^{phy}$ - Phytoplankton Respiration - Phosphorus

Units	Output Variable Name
mg/L/d	WQ_DIAG_PHY_NAME_RESP_P_MG_L_D
mmol/m ³ /d	WQ_DIAG_PHY_NAME_RESP_P_MMOL_M3_D

Science: Equation H.11

Core Constituent Model: Phytoplankton - Basic

The flux of phosphorus from phytoplankton as a result of energy consumption (referred to as true respiration). It is typically seen as a night time phytoplanktonic process but can also occur during the day. Values are only negative. Multiply by cell volume (m^3) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be lost via true respiration in that interval

$F_{N\text{-uptake}}^{\text{phy}}$ - Phytoplankton Primary Productivity - Nitrogen

Units	Output Variable Name
mg/L/d	WQ_DIAG_PHY_NAME_PRIM_PROD_N_MG_L_D
mmol/ m^3 /d	WQ_DIAG_PHY_NAME_PRIM_PROD_N_MMOL_M3_D

Science: Equation J.2, Equation J.4

Core Constituent Model: Phytoplankton - Basic, Phytoplankton - Advanced

The flux of nitrogen to phytoplankton as a result of productivity, without accounting for respiration, for a phytoplankton group. Also referred to as growth or gross primary productivity, and typically associated with daytime phytoplankton photosynthesis. Values are only positive. Multiply by cell volume (m^3) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be taken up via productivity in that interval. This diagnostic variable name is used for both basic and advanced phytoplankton groups, even though the method to compute uptake differs between the two

$F_{P\text{-uptake}}^{\text{phy}}$ - Phytoplankton Primary Productivity - Phosphorus

Units	Output Variable Name
mg/L/d	WQ_DIAG_PHY_NAME_PRIM_PROD_P_MG_L_D
mmol/ m^3 /d	WQ_DIAG_PHY_NAME_PRIM_PROD_P_MMOL_M3_D

Science: Equation J.7, Equation J.8

Core Constituent Model: Phytoplankton - Basic, Phytoplankton - Advanced

The flux of phosphorus to phytoplankton as a result of productivity, without accounting for respiration, for a phytoplankton group. Also referred to as growth or gross primary productivity, and typically associated with daytime phytoplankton photosynthesis. Values are only positive. Multiply by cell volume (m^3) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be taken up via productivity in that interval. This diagnostic variable name is used for both basic and advanced phytoplankton groups, even though the method to compute uptake differs between the two

$F_{\text{sedmtn-N(computed)}}^{\text{phy}}$ - Phytoplankton Sedimentation - Nitrogen

Units	Output Variable Name
mg/L/d	WQ_DIAG_PHY_NAME_SEDMTN_N_MG_L_D
mmol/ m^3 /d	WQ_DIAG_PHY_NAME_SEDMTN_N_MMOL_M3_D

Science: Equation H.14, Equation H.15

Core Constituent Model: Phytoplankton - Basic, Phytoplankton - Advanced

The flux of phytoplankton nitrogen into the sediments as a result of settling for a phytoplankton group. Values are only losses and are only negative. Multiply by cell volume (L or m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be lost to settling in that interval. This diagnostic variable name is used for both basic and advanced phytoplankton groups, even though the method to compute uptake differs between the two. Although often thought of as being a per area (per m²) loss, the volumetric units of this diagnostic (per L or m³) have been chosen deliberately for consistency with other analogous volumetric losses such as mortality. This is intended to assist in simplifying post processing

$F_{sedmntn-P}^{phy}$ - Phytoplankton Sedimentation - Phosphorus

Units	Output Variable Name
mg/L/d	WQ_DIAG_PHY_NAME_SEDMTN_P_MG_L_D
mmol/m ³ /d	WQ_DIAG_PHY_NAME_SEDMTN_P_MMOL_M3_D

Science: Equation [H.16](#), Equation [H.17](#)

Core Constituent Model: Phytoplankton - Basic, Phytoplankton - Advanced

The flux of phytoplankton phosphorus into the sediments as a result of settling for a phytoplankton group. Values are only losses and are only negative. Multiply by cell volume (L or m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be lost to settling in that interval. This diagnostic variable name is used for both basic and advanced phytoplankton groups, even though the method to compute uptake differs between the two. Although often thought of as being a per area (per m²) loss, the volumetric units of this diagnostic (per L or m³) have been chosen deliberately for consistency with other analogous volumetric losses such as mortality. This is intended to assist in simplifying post processing

F_{C-excr}^{phy} - Phytoplankton Excretion

Units	Output Variable Name
mg/L/d	WQ_DIAG_PHY_NAME_EXCR_MICG_L_D
mmol/m ³ /d	WQ_DIAG_PHY_NAME_EXCR_MMOL_M3_D

Science: Equation [K.1](#)

Core Constituent Model: Phytoplankton - Basic

The flux of carbon from phytoplankton as a result of excretion for a phytoplankton group. Values are only negative. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be lost via excretion in that interval

F_{C-mort}^{phy} - Phytoplankton Mortality

Units	Output Variable Name
mg/L/d	WQ_DIAG_PHY_NAME_MORT_MICG_L_D
mmol/m ³ /d	WQ_DIAG_PHY_NAME_MORT_MMOL_M3_D

Science: Equation [K.2](#)

Core Constituent Model: Phytoplankton - Basic

The flux of carbon from phytoplankton as a result of mortality for a phytoplankton group. Values are only negative. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be lost via mortality in that interval

F_{N-excr}^{phy} - Phytoplankton Excretion - Nitrogen

Units	Output Variable Name
mg/L/d	WQ_DIAG_PHY_NAME_EXCR_N_MG_L_D
mmol/m ³ /d	WQ_DIAG_PHY_NAME_EXCR_N_MMOL_M3_D

Science: Equation [K.3](#)

Core Constituent Model: Phytoplankton - Basic

The flux of nitrogen from phytoplankton as a result of excretion for a phytoplankton group. Values are only negative. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be lost via excretion in that interval

F_{N-mort}^{phy} - Phytoplankton Mortality - Nitrogen

Units	Output Variable Name
mg/L/d	WQ_DIAG_PHY_NAME_MORT_N_MG_L_D
mmol/m ³ /d	WQ_DIAG_PHY_NAME_MORT_N_MMOL_M3_D

Science: Equation [K.4](#)

Core Constituent Model: Phytoplankton - Basic

The flux of nitrogen from phytoplankton as a result of mortality for a phytoplankton group. Values are only negative. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be lost via mortality in that interval

F_{P-excr}^{phy} - Phytoplankton Excretion - Phosphorus

Units	Output Variable Name
mg/L/d	WQ_DIAG_PHY_NAME_EXCR_P_MG_L_D
mmol/m ³ /d	WQ_DIAG_PHY_NAME_EXCR_P_MMOL_M3_D

Science: Equation [K.5](#)

Core Constituent Model: Phytoplankton - Basic

The flux of phosphorus from phytoplankton as a result of excretion for a phytoplankton group. Values are only negative. Multiply by cell volume (m³) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be lost via excretion in that interval

F_{P-mort}^{phy} - Phytoplankton Mortality - Phosphorus

Units	Output Variable Name
mg/L/d	WQ_DIAG_PHY_NAME_MORT_P_MG_L_D
mmol/m ³ /d	WQ_DIAG_PHY_NAME_MORT_P_MMOL_M3_D

Science: Equation [K.6](#)

Core Constituent Model: Phytoplankton - Basic

The flux of phosphorus from phytoplankton as a result of mortality for a phytoplankton group. Values are only negative. Multiply by cell volume (m^3) and time interval of interest (seconds / 86400) to compute the mass (or moles) that would be lost via mortality in that interval

$F_{sed(computed)}^{FRPAds}$ - Adsorbed FRP Sedimentation Rate

Units	Output Variable Name
mg/L/d	WQ_DIAG_FRP_ADS_SEDMTN_FLUX_MG_L_D
mmol/ m^3 /d	WQ_DIAG_FRP_ADS_SEDMTN_FLUX_MMOL_M3_D

Currently unused and reported as zero. Will be activated in future releases

F_{resus}^{FRPads} - Adsorbed FRP Resuspension Rate

Units	Output Variable Name
mg/L/d	WQ_DIAG_FRP_ADS_RESUS_FLUX_MG_L_D
mmol/ m^3 /d	WQ_DIAG_FRP_ADS_RESUS_FLUX_MMOL_M3_D

Currently unused and reported as zero. Will be activated in future releases

$F_{ads(computed)}^{FRP}$ - FRP Adsorption Rate

Units	Output Variable Name
mg/L/d	WQ_DIAG_FRP_ADSORPTION_RATE_MG_L_D
mmol/ m^3 /d	WQ_DIAG_FRP_ADSORPTION_RATE_MMOL_M3_D

Currently unused and reported as zero. Will be activated in future releases

F_{mor}^{pth} - Pathogen Mortality

Output Variable Name: WQ_DIAG_PATH_NAME_MORTALITY_CFU_100ML_D

Units: CFU/100mL/d

Science: Equation [N.1](#)

Core Constituent Model: Pathogen - Free

The flux of pathogens from alive to dead, as a result of natural (dark death) mortality. This flux includes the mortality of attached pathogens, if they are simulated. This is not the inactivation flux due to irradiation.

F_{invn}^{pth} - Pathogen Inactivation

Output Variable Name: WQ_DIAG_PATH_NAME_LIGHT_CFU_100ML_D

Units: CFU/100mL/d

Science: Equation [N.3](#)

Core Constituent Model: Pathogen - Free

The flux of pathogens from alive to dead, as a result of irradiation. This flux includes the inactivation of attached pathogens, if they are simulated. This is not the dark death flux due to mortality.

F_{att}^{pth} - Pathogen Attachment

Output Variable Name: WQ_DIAG_PATH_NAME_ATTACHMENT_CFU_100ML_D

Units: CFU/100mL/d

Science: Equation [N.4](#)

Core Constituent Model: Pathogen - Attached

The flux of pathogens from free to attached, if attached pathogens are simulated. A positive (negative) flux is attachment (detachment)

$F_{sedmnt(computed)}^{pth_a}$ - Pathogen Alive Sedimentation

Output Variable Name: WQ_DIAG_PATH_NAME_ALIVE_SEDMTN_CFU_100ML_D

Units: CFU/100mL/d

Science: Equation [N.6](#)

Core Constituent Model: Pathogen - Free

The flux of alive pathogens into the sediments as a result of settling for a pathogen group. Values are only losses and are only negative. Multiply by volume and time interval of interest (seconds / 86400) to compute the CFU that would be lost to settling in that interval. Although often thought of as being a per area (per m²) loss, the volumetric units of this diagnostic have been chosen deliberately for consistency with other analogous volumetric losses such as mortality. This is intended to assist in simplifying post processing

$F_{sedmnt(computed)}^{pth_d}$ - Pathogen Alive Sedimentation

Output Variable Name: WQ_DIAG_PATH_NAME_DEAD_SEDMTN_CFU_100ML_D

Units: CFU/100mL/d

Science: Equation [N.6](#)

Core Constituent Model: Pathogen - Free

The flux of dead pathogens into the sediments as a result of settling for a pathogen group. Values are only losses and are only negative. Multiply by volume and time interval of interest (seconds / 86400) to compute the CFU that would be lost to settling in that interval. Although often thought of as being a per area (per m²) loss, the volumetric units of this diagnostic have been chosen deliberately for consistency with other analogous volumetric losses such as mortality. This is intended to assist in simplifying post processing

$F_{sedmnt(computed)}^{pth_t}$ - Pathogen Attached Sedimentation

Output Variable Name: WQ_DIAG_PATH_NAME_ATTCHD_SEDMTN_CFU_100ML_D

Units: CFU/100mL/d

Science: Equation [N.7](#)

Core Constituent Model: Pathogen - Attached

The flux of attached pathogens into the sediments as a result of settling for a pathogen group. Values are only losses and are only negative. Multiply by volume and time interval of interest (seconds / 86400) to compute the CFU that would be lost to settling in that interval. Although often thought of as being a per area (per m²) loss, the volumetric units of this diagnostic have been chosen deliberately for consistency with other analogous volumetric losses such as mortality. This is intended to assist in simplifying post processing

$F_{growth(computed)}^{pth_a}$ - Pathogen Growth

Output Variable Name: WQ_DIAG_PATH_NAME_GROWTH_CFU_100ML_D

Units: CFU/100mL/d

Currently unused and reported as zero. Will be activated in future releases

$[PTH]^{TOT}$ - Total Pathogens

Output Variable Name: WQ_DIAG_PATH_NAME_TOTAL_CFU_100ML_D

Units: CFU/100mL

Science: Equation [N.8](#)

Core Constituent Model: Pathogen - Free

The sum of alive, dead and attached (if the latter is simulated) pathogens for a pathogen group



Q Mass Conservation Model

Q.1 Intent

The TUFLOW FV Water Quality (WQ) Module is supported by a downloadable model suite that is intended to provide users with simple three dimensional models that can be used to:

- Assess and understand WQ Module mass conservation performance
- Support exploration of the features and behaviour of the WQ Module
- Use as templates for building water quality control files for other simulations

The suite does not need a licence to execute with either existing or altered water quality parameters.

This Appendix provides information related to the mass conservation model. The model suite can be run on either Windows or linux, however this document describes only the Windows execution process.

Q.2 Description

The mass conservation model is configured as follows.

- General
 - 1 month (745 hours) duration
 - Includes salinity, temperature (and heat calculations), sediment and varying numbers of water quality computed variables
 - 15 minute output
 - 15 minute water quality simulation timestep
 - Designed to mimic a deep lake that cools over an autumnal period
- Geometry
 - Four three-dimensional flat bottomed columns, with the same bed elevation
 - Lateral cell areas each of approximately 10 km²
 - Depth of 21 metres
 - 20 vertical layers of variable thickness, with 17 fixed and 3 sigma (which span the top portion of the water column)
- Boundary conditions
 - No inflows, outflows or other flow boundaries
 - Meteorological boundaries applied
 - * Hourly timestep
 - * Typical mid latitude autumnal conditions, with rainfall included
- Water quality parameterisation
 - Parameters are set to be generally within expected ranges

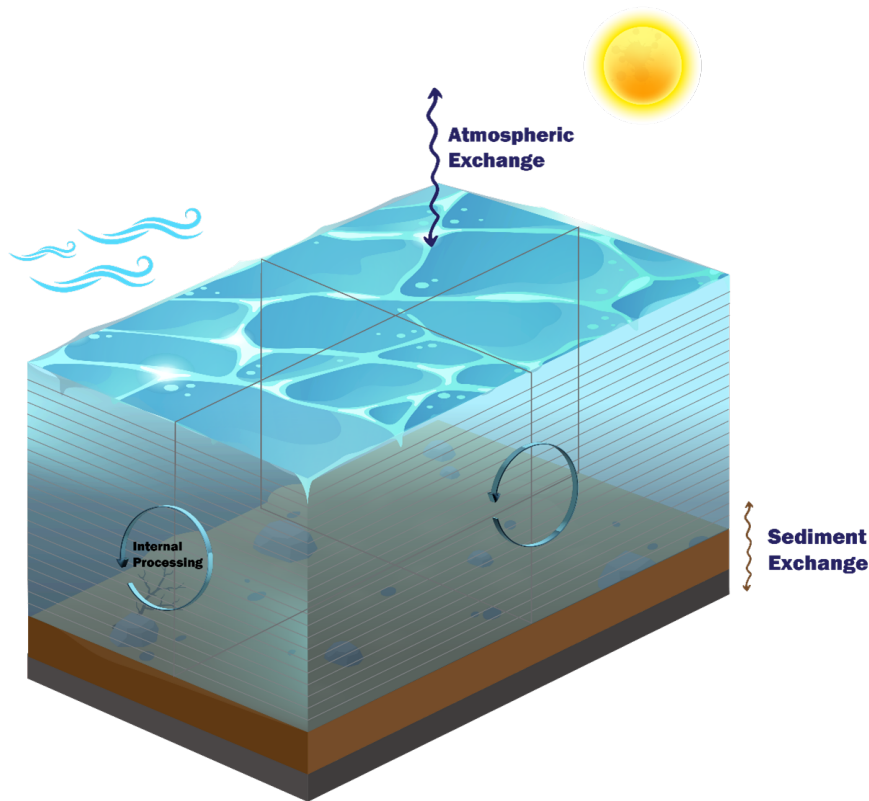


Figure Q.1: WQ Module Mass Conservation Model

This setup of essentially stationary water is designed to be challenging for mass conservation. In particular, the exclusion of external flow boundaries (that can reset or overwhelm internal process calculations) is deliberate. These conditions might mimic a low rainfall lacustrine environment.

Q.3 Model suite

The mass conservation model suite comprises three (3) related models. The three models increase in a configurational complexity that matches the three currently available water quality simulation classes. These are (with links to the relevant manual sections):

- [Water Quality Simulation Class == DO](#) (Section 3.1)
- [Water Quality Simulation Class == Inorganics](#) (Section 3.2)
- [Water Quality Simulation Class == Organics](#) (Section 3.3)

The mass balance models can be downloaded (see Section Q.5) and run as is. The associated mass balance output files can then be interrogated by the user to assess mass balance using any spreadsheet package.

Q.4 Calculations

The primary calculation used to assess mass conservation for each computed variable X is a comparison between two independent calculations of instantaneous mass in the model as follows:

$$X_{mb}(t) = 100 \times \frac{X_{mp}(t) - X_{mi}(t)}{X_{mi}(t)} \quad (\text{Q.1})$$

where $X_{mb}(t)$ is the percentage difference (column 'MF_PCT_ERROR' in mass flux output csv files) between two methods of computing the mass of computed variable X in the domain:

- $X_{mp}(t)$: Progressively modifying the initial domain mass by adding to it the sum of the relevant fluxes F_i at each timestep t (column 'MF_WQ_MASS' in mass flux output csv files). No resetting of this calculation occurs - it is designed (stringently) such that any mass conservation errors will accumulate in time
- $X_{mi}(t)$: Multiplying the reported concentrations of X in cell j of volume V_j and integrating over the entire model domain at each timestep t (column 'FV_WQ_MASS' in mass flux output csv files). This mass is reset at each timestep and corresponds to the mass reported by TUFLOW FV

$X_{mp}(t)$ and $X_{mi}(t)$ are computed as per Equation Q.2. $F_i(t)$ are the relevant fluxes for X (up to a total number of $i = NF$ fluxes) and are converted from per area (or per volume) and per time amounts to mass amounts. The number of cells in the domain is NC , and $[X]_j(t)$ is the concentration of computed variable X in cell j at time t . The model contains sigma layers and as such V_j may be time varying.

$$\left. \begin{aligned} X_{mp}(t) &= \sum_{j=1}^{NC} [X]_j(0) \times V_j(0) + \sum_{i=1}^{NF} F_i(t) \\ X_{mi}(t) &= \sum_{j=1}^{NC} [X]_j(t) \times V_j(t) \end{aligned} \right\} \quad (\text{Q.2})$$

None of the quantities above need to be computed by the user - all are output directly in files created when the MassBalance output block is called (see Section 4.9.2):

```
Output == MassBalance
  Output Interval == 900.00
End Output
```

As a general note, reported fluxes often need to be interpreted with care in mass conservation analyses. This is because fluxes are reported as instantaneous values, and are not integrated or accumulated between overall model output file writing timesteps. For example, if water quality calculations are undertaken every 15 minutes but outputs are written every hour, then several water quality calculations are undertaken between reporting. Whilst the hourly output water quality concentrations will correctly reflect the cumulative action of fluxes at every 15 minute increment, the on-the-hour output fluxes will be instantaneous, and equal to those that happen to be occurring at the hourly output time. They will not necessarily be reflective of the fluxes that occurred over the course of the preceding hour. Using these fluxes in mass conservation calculations can therefore lead to spurious outcomes. One solution to this matter is to set the output and water quality (and boundary condition update) timesteps to be the same in mass conservation analyses, noting that this may however generate large output files.

Q.5 Access and execution

Q.5.1 Access

To download the mass conservation model:

1. Download the zip from the TUFLOW website by clicking [here](#) (under Example / Demo Models section)
2. Unzip the model in a convenient location. For the purposes of this description, the location of the mass conservation model suite is assumed to be:
 - i. 'C:\TUFLOWFV\Models\'

The above steps will create a subfolder called 'wqm' within the chosen folder location. Within this wqm subfolder will be another subfolder called mass_conservation_model. This is where the mass conservation model resides.

Q.5.2 Execution

Unzipping the above will generate the folder structure within C:\TUFLOWFV\Models\wqm\mass_conservation_model\ with subfolders as follows:

- bc_dbase: Boundary condition data

- `model1`: Model geometry and related data
- `results`: Model results (will be empty on initial download)
- `runs`: TUFLOW FV hydrodynamic and sediment transport control files
- `wqm`: TUFLOW FV WQ Module control files

After navigating to the runs folder, the mass conservation model can now be executed via a windows command line as normal - the included 'run_all.bat' batch file will execute all three models, once the path to the TUFLOW executable has been set. Subsequently generated mass balance outputs can be viewed in any spreadsheet package, or more advanced post processing platforms if desired. Suggested plotting approaches are provided in Section 4.9.2.

Q.6 Example results

The following figures provide an example of the progressively more complex dissolved oxygen dynamics that characterise the DO, Inorganics and Organics Simulation Classes. The top pane in each figure is a timeseries of the total mass of dissolved oxygen and the bottom pane plots the cumulative fluxes written to the respective '*_MASSBALANCE_DISS_OXYGEN_MG_L.csv' mass balance output files. The number of Turnovers is also plotted on the secondary vertical axis of the lower plot, in orange. No post processing has been performed.

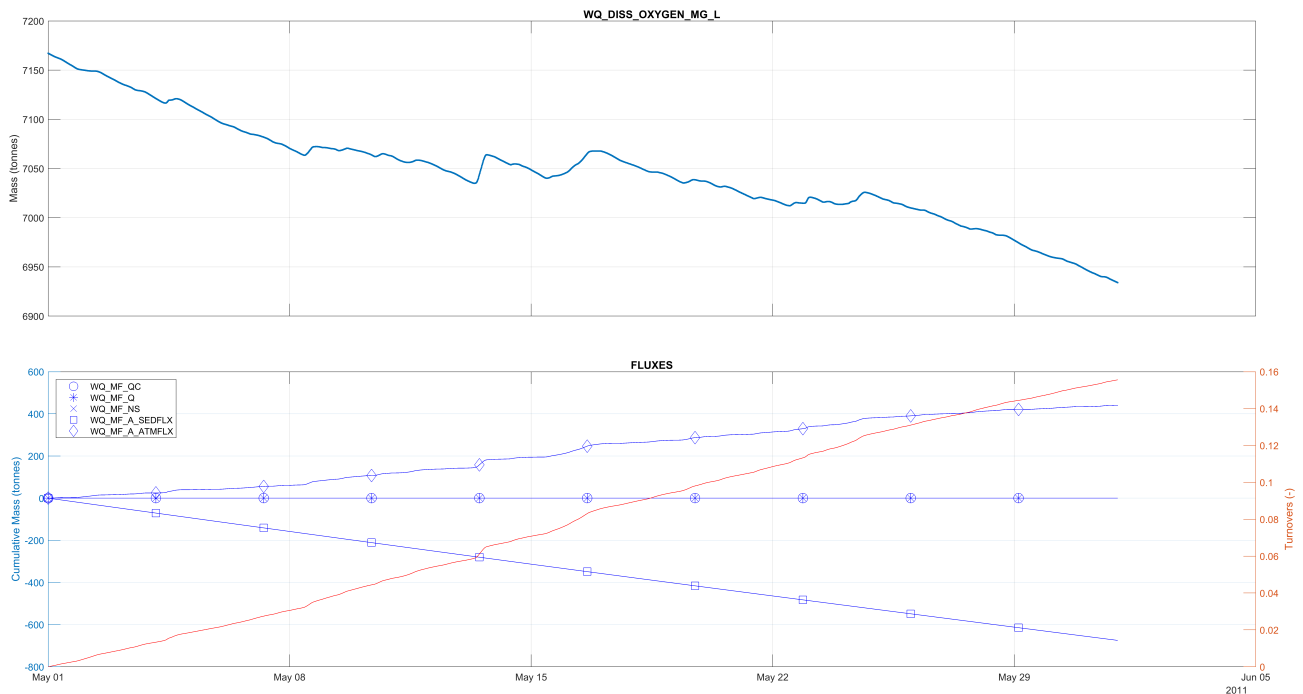


Figure Q.2: Dissolved oxygen mass balance output: DO Simulation Class. Percentage error: 0.006%

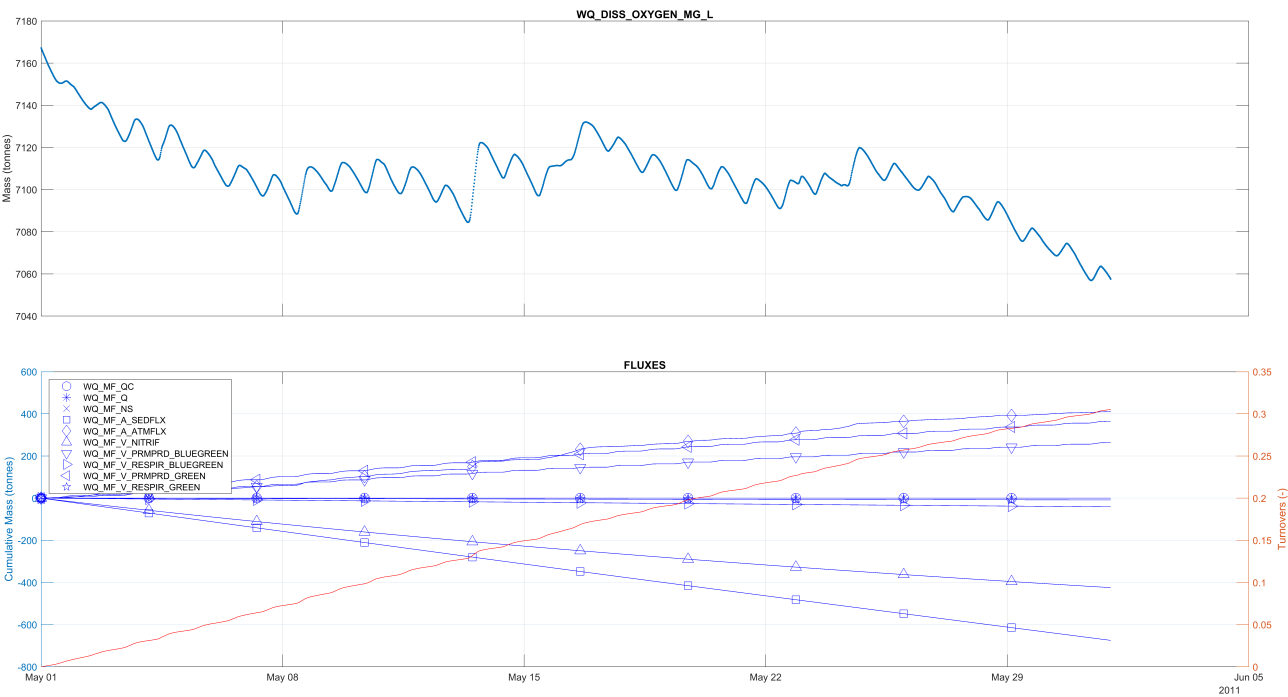


Figure Q.3: Dissolved oxygen mass balance output: Inorganics Simulation Class. Percentage error: 0.017%

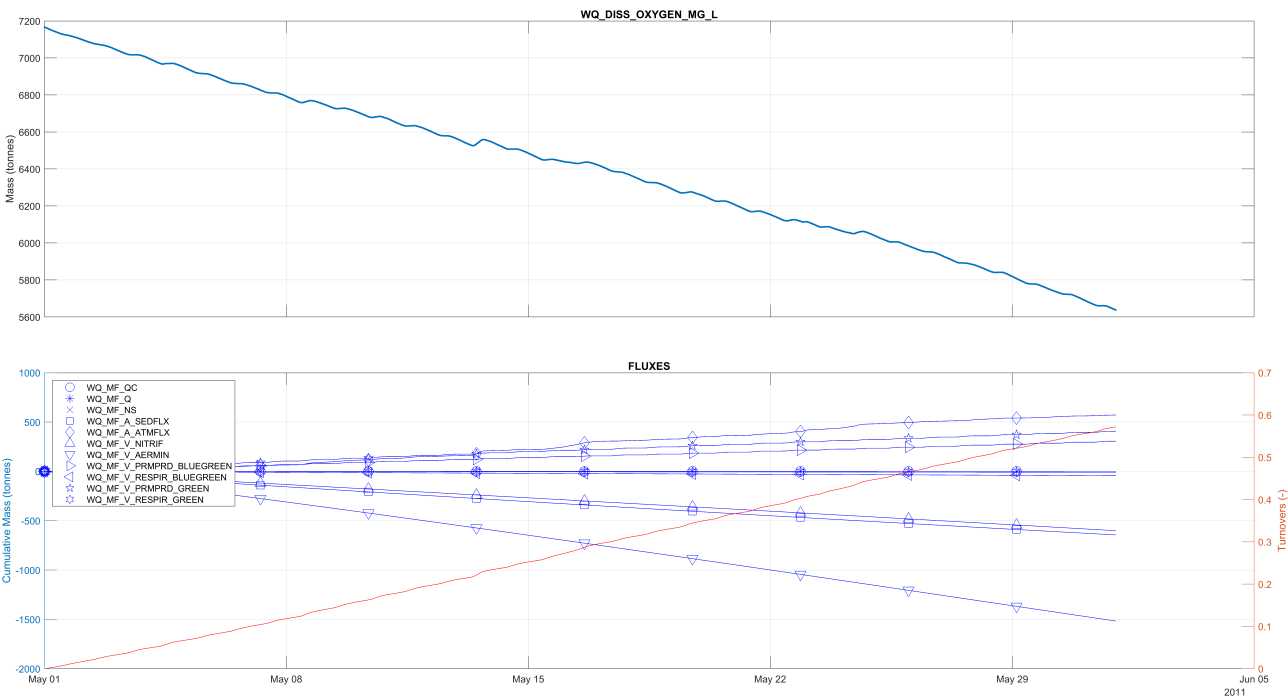


Figure Q.4: Dissolved oxygen mass balance output: Organics Simulation Class. Percentage error: 0.022%