



Computational Aquatic Ecosystem Dynamics Model: CAEDYM v2

v2.3 Science Manual

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January 16, 2006

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Preface

The first generation of CAEDYM was initiated and developed by Michael Herzfeld and David Hamilton. Later revisions and developments were conducted by Barbara Robson and Dirk Slawinski. Following numerous applications, and based on advances in computational power, many components of CAEDYM were reorganised and rewritten by Matthew Hipsey with Jose Romero and Jason Antenucci, which ultimately produced the CAEDYM v2 series in 2003. Since then, numerous additions and developments have been made to this and public releases of CAEDYM v2.1 (2004) and now v2.2 (2005) have been made. From its initial conception, scientific direction, guidance and provision of funds for ongoing developments and improvements have come from Prof. Jörg Imberger.

CAEDYM has evolved significantly since its original inception. However, it has always aimed to be a generic and flexible tool for use in a range of surface water environments. It has now been applied to hundreds of lakes, reservoirs and other surface waters around the globe for a variety of applications ranging from nutrient cycling studies, algal succession studies, food-web investigations, pathogen dynamics investigations, suspended solids studies, and toxic metal studies. CAEDYM is now used by research scientists, consultant engineers, and government agencies for investigative and routine management applications. Recently, it has also been used in several online real-time management applications as part of a larger aquatic decision support system.

It is programmed in Fortran-90 and runs on Macintosh, Linux, Unix and Windows operating systems, and the source-code is made freely-available to scientists interested in modifying or developing the code. The purpose of this manual is to outline the scientific theory behind the various CAEDYM modules, and to provide a detailed account of the algorithms CAEDYM is using. Readers are also directed to the accompanying *CAEDYM v2.2 User Manual*, which covers detailed technical information on how to configure, run, and analyse a CAEDYM simulation.

Modellers interested in discussing topics covered in this Science Manual are directed to the online user community at: http://www.cwr.uwa.edu.au/services/model_forum/

Introduction

1.1 Overview

CAEDYM is an aquatic ecological model designed to be readily linked to hydrodynamic models, which currently includes DYRESM, DYRIM and ELCOM. DYRESM is a one-dimensional model used for predicting vertical density stratification in lakes and reservoirs (Gal et al., 2003; Yeates and Imberger, 2004). It has been coupled previously with process representations of biogeochemical processes (DYRESM-WQ: Hamilton and Schladow (1997); Schladow and Hamilton (1997); Hamilton et al. (1995); Schladow and Hamilton (1995)). ELCOM is a three-dimensional hydrodynamic model applicable to lakes (Hodges et al., 2000), reservoirs (Romero and Imberger, 2003; Romero et al., 2003), estuaries (Robson and Hamilton, 2004; Chan et al., 2002) and the coastal ocean (Spillman et al., 2005; Hillmer and Imberger, 2005). Recently, CAEDYM has been coupled to DYRIM (a quasi-2D Lagrangian river-floodplain model; Devkota and Imberger (2005)) to simulate biogeochemical processing in rivers. The coupling between CAEDYM and the hydrodynamic driver is dynamic; in particular, the thermal structure of the water body is dependent on the water quality concentrations by feeding back through water clarity.

One of the objectives during CAEDYM development was to allow flexible ecological configuration that could be tailored for specific applications, though major elemental cycling and at least one algal group is compulsory. Hence, the model includes comprehensive process representation of the C, N, P, Si and DO cycles, several size classes of inorganic suspended solids, and phytoplankton dynamics. Numerous optional biological and other state variables can also be configured. Hence, CAEDYM is more advanced than traditional N-P-Z models, as it is a general biogeochemical model that can resolve species- or group-specific ecological interactions. CAEDYM operates on any sub-daily time step to resolve algal processes (diurnal photosynthesis and nocturnal respiration), and is generally run at the same time interval as the hydrodynamic model. Algorithms for salinity dependence are included so that a diverse range of aquatic settings can be simulated. The user can prescribe whether the simulation is for freshwater, estuaries or coastal waters, since many of the algorithms have been developed to include a salinity dependence. With specification of the nature of the waterbody (i.e. fresh, estuarine or marine), internal checks in the model are then activated to ensure that salinity dependence is maintained (for an estuarine case) or removed (for a freshwater or marine water case). Further details of salinity dependence are given later in the process descriptions.

The major biogeochemical state variables in CAEDYM are given in Figure 1.1. A simple configuration file exists that allows users to customise the model elements that should be included within any simulation. An input file for parameters can also be adjusted rather than modifying the source code, but inevitably, a small number of users will have specific variables of interest which have not been represented in CAEDYM, thus necessitating some modification to the source code.

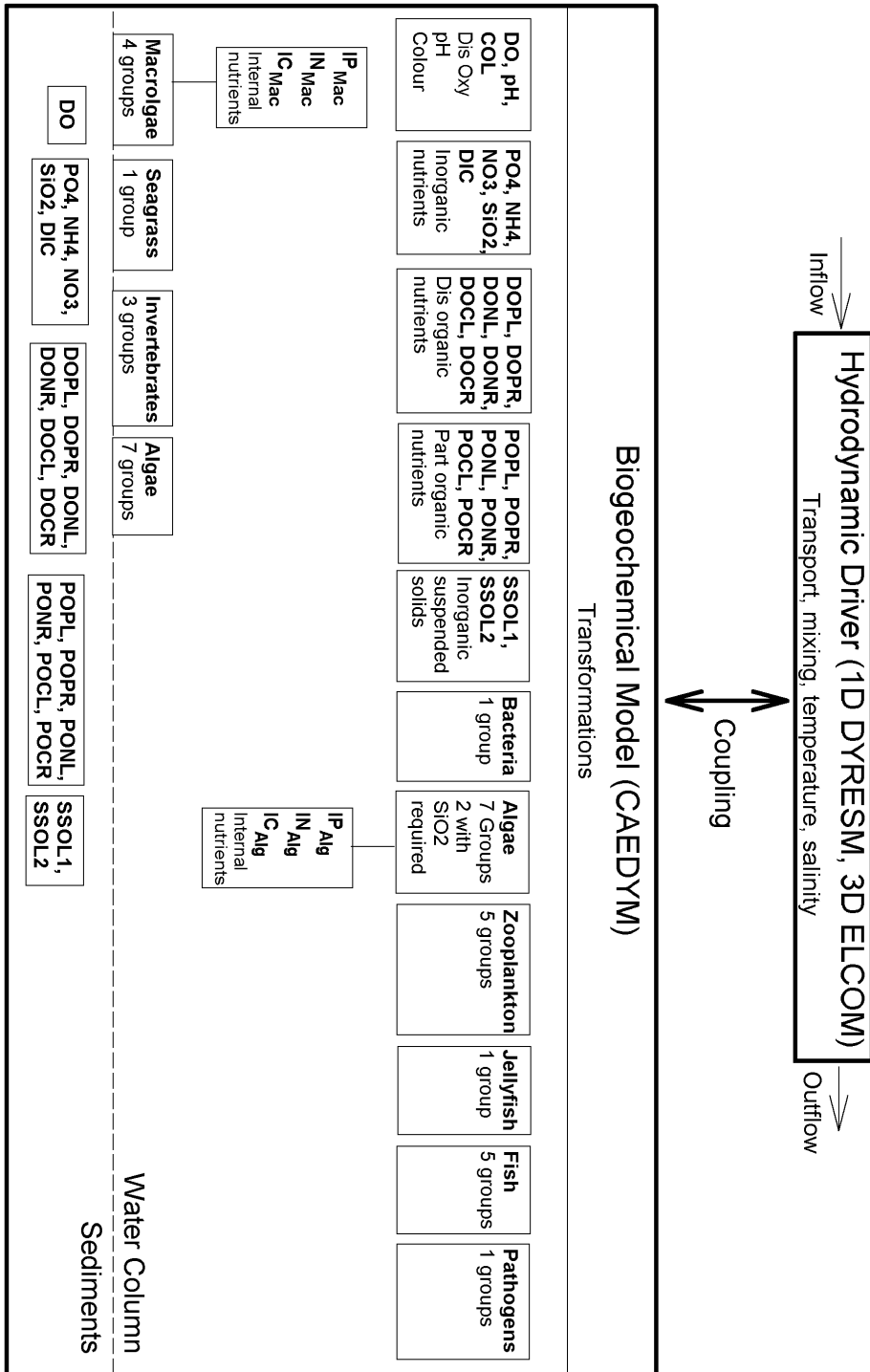


Figure 1.1 Overview of CAEDYM state variables showing the water column, benthic and sediment components.

1.2 Simulated Variables

CAEDYM simulates the C , N , P , DO , and Si cycles along with inorganic suspended solids, phytoplankton, and optional biotic compartments such as zooplankton, fish, bacteria and others Figure (1.1).

1.2.1 Light Incident shortwave radiation is supplied by the hydrodynamic driver, where it is used for surface thermodynamics calculations, to CAEDYM. For primary production, the shortwave (280-2800 nm) intensity at the surface is converted to the photosynthetically active component (PAR) based on the assumption that 45% of the incident spectrum lies between 400-700 nm (Jellison and Melack, 1993). PAR is assumed to penetrate into the water column according to the Beer-Lambert Law with the light extinction coefficient dynamically adjusted to account for variability in the concentrations of algal, inorganic and detrital particulates, and dissolved organic carbon levels. The ultra-violet component of the incident light can also be used for looking at pathogen inactivation and organic matter photolysis.

1.2.2 Inorganic Particles Two inorganic particle groups (SS) can optionally be included within the simulation, with each group assigned a unique diameter and density, and modelled as a balance between resuspension and settling. Adsorption and desorption of aqueous-phase FRP and NH_4 onto inorganic particles (PIP and PIN) can also be configured. Particle settling is modelled on the basis of Stokes Law.

1.2.3 Sediments and Resuspension CAEDYM maintains mass balance of C , N , P , Si , SS and all other simulate variables in both the water column and a single sediment layer. The main aim in this development stage of CAEDYM was to provide a complete description of the dominant pools and fluxes in the water column with only sufficient complexity of the sediments to maintain mass conservation. The sediment fluxes of dissolved inorganic and organic nutrients are based on empirical formulations that account for environmental sensitivities and require laboratory and field studies to establish parameter values. The relative proportions of the particulate components of the sediments are simulated to determine the appropriate resuspension parameters for each component.

Resuspension of inorganic (SS) and organic particles (POM) from the sediment-water interface require a number of parameters including the critical shear stress and the resuspension rate constant. The composition of the sediments is established in the CAEDYM initial conditions file for the particulate organic matter (POC , PON , POP); and each of the inorganic suspended solids state variables (SS_s). The initial $C : N : P$ ratio of the organic component of the sediments is used throughout the simulation for the composition of particles that are resuspended.

1.2.4 Dissolved Oxygen DO dynamics within CAEDYM include atmospheric exchange, the sediment oxygen demand (SOD), microbial use during organic matter mineralization and nitrification, photosynthetic oxygen production and respiratory oxygen consumption, and respiration by other optional biotic components. Atmospheric

exchange is based on the model of Wanninkhof (1992) and the flux equation of Riley and Skirrow (1974). A simple static sediment oxygen demand model is currently employed within CAEDYM that varies as a function of the overlying water temperature and dissolved oxygen levels. Microbial activity facilitates the breakdown of organic carbon (in particular, *DOC*) to CO_2 , and a stoichiometrically equivalent amount of oxygen is removed. The process of nitrification also requires oxygen that is dependent on the stoichiometric factor for the ratio of oxygen to nitrogen ($Y_{O_2:N}$) and the half-saturation constant for the effect of oxygen limitation (K_{NIT}). Photosynthetic oxygen production and respiratory oxygen consumption is summed over the number of simulated phytoplankton groups.

1.2.5 Carbon, Nitrogen, Phosphorus and Silica Both the inorganic and organic, and dissolved and particulate forms of *C*, *N* and *P* are modelled explicitly along the degradation pathway of *POM* to *DOM* to dissolved inorganic matter (*DIM*). The nitrogen cycle includes the additional processes of denitrification, nitrification and N_2 fixation that are not in the carbon and phosphorus cycles. N_2 levels are not tracked by CAEDYM.

The silica cycle is simpler and includes the processes of biological uptake of dissolved *Si* (SiO_2) by diatoms into the internal *Si* (*ISi*) pool, dissolved sediment fluxes of SiO_2 , diatom mortality directly into the SiO_2 sediment pool, settling of *ISi*, and resuspension of *ISi*. This relatively simple representation assumes that diatom frustules rapidly settle into the sediments and the organic silica is rapidly mineralized.

The *DIC* balance additionally includes atmospheric fluxes of CO_2 that are based on the difference between the atmospheric and water column values of pCO_2 . The transfer is calculated according to Wanninkhof (1992) with the solubility product of CO_2 estimated from Weiss (1974). To estimate the CO_2 fraction of the *DIC* pool, the carbonate buffer system, *pH* and alkalinity are modelled following Butler (1982). Gaseous and aqueous phase CO_2 values are related by Henrys Law for calculation of pCO_2 .

1.2.6 Phytoplankton Dynamics Seven phytoplankton groups are configurable within CAEDYM that are generic except for several diatom groups, which include internal silica stores. Algal biomass can be simulated either in units of *chl*a ($\mu g\ chl\ a\ L^{-1}$) or carbon ($mg\ C\ L^{-1}$). For each phytoplankton group, the maximum potential growth rate at 20C is multiplied by a temperature function and the minimum value of expressions for limitation by light, phosphorus, nitrogen and silica when diatoms are considered. Phytoplankton may also be grazed upon by zooplankton, fish, and clams.

Light limitation on phytoplankton growth can be configured to be subject to photoinhibition or to be non-photoinhibited. In the absence of significant photoinhibition, the model of Webb et al. (1974) is used to quantify the fractional limitation of the maximum potential rate of carbon fixation if light saturation behavior was absent (Talling, 1957), and the equations are analytically integrated with respect to depth. For the case of photoinhibition, the light saturation value of maximum production uses a depth integral.

There are two options to model the C , P , and N dynamics within the algal groups: a constant nutrient to $chl a$ ratio, or dynamic intracellular stores. For the first model (Romero et al., 2003), a simple Michaelis-Menten equation is used to model nutrient limitation with a half-saturation constant for the effect of external nutrient concentrations on the growth rate as for SiO_2 in this application. Metabolic loss of nutrients from mortality and excretion is proportional to the constant internal nutrient to $chl a$ ratio multiplied by the loss rate and the fraction of excretion and mortality that returns to the detrital pool. The latter model uses dynamic intracellular stores that are able to regulate growth with the model of Droop (1974). This model allows for the phytoplankton to have variable internal nutrient concentrations with dynamic nutrient uptake bounded by minimum and maximum values. Nutrient losses through mortality and excretion for the internal nutrient model are similar to the simple model described above, except that the dynamically calculated internal nutrient concentrations are used.

For diatom groups modelled in CAEDYM, silica processes that are modelled include uptake of dissolved silica, an internal store of silica, and loss through mortality and excretion. The silica limitation function for diatoms is similar to the constant internal cases for nitrogen and phosphorus. During diatom senescence, silica loss is considered to be particulate (i.e. the diatom frustules) and to settle directly to the sediments.

Loss terms for respiration, natural mortality and excretion are modelled with a single respiration rate coefficient. This loss rate is then divided into the pure respiratory fraction and losses due to mortality and excretion. The constant f_{DOM} is the fraction of mortality and excretion to the dissolved organic pool with the remainder into the particulate organic pool.

There are 4 models in CAEDYM for phytoplankton migration and settling including constant settling, Stokes law settling based on dynamically calculated cell density, migration without photoinhibition, and migration with photoinhibition. Phytoplankton that settle into the sediments are assumed to persist for a user-defined period (usually 24 hours) when the phytoplankton may be resuspended. If the phytoplankton do not re-enter the water column, their biomass enters the respective nutrient pools of the sediment.

1.2.7 Bacteria Bacterial biomass may also be modelled explicitly, thereby allowing dynamic prediction of organic matter mineralisation. The bacteria are prescribed a fixed $C : N : P$ ratio that is constant over the course of the simulation. They are assumed to primarily receive nutrients from the dissolved organic matter pool. The incoming nutrients are converted to CO_2 , NH_4 and FRP and released back to the water column. Under low nutrient conditions they may not be able to satisfy their $C : N : P$ ratio and their growth and ability to mineralise organic matter will be limited.

The bacterial sub-model was implemented to account for the role of heterotrophic micro-organisms which are responsible for decaying detrital material produced by phytoplankton and zooplankton. A special oxygen dependence is included that accounts for bacterial activity under aerobic and anaerobic conditions. As well as the

oxygen availability in the water, the decomposition of particulate organic matter also has a dependence on the bacterial biomass. Zooplankton are also able to graze on bacteria and incorporate their C , N and P .

1.2.8 Zooplankton CAEDYM assumes each zooplankton group has a fixed $C : N : P$ ratio and depending on the C:N:P ratio of the various food sources, the groups balance their internal concentration by excretion of labile dissolved organic matter. The grazing preference of each group is user defined, and can be for any of the simulated algal, zooplankton, bacterial or detrital groups. Faecal pellets can also be specified as either hard, soft or in between, and lost to the sediment or returned to the detrital pool.

1.2.9 Higher Biology CAEDYM has the facility to model higher organisms such as fish, jellyfish, and benthic organisms including macroalgae, benthic macroinvertebrates and clams/mussels.

1.2.10 Pathogens and Microbial Indicator Organisms CAEDYM has an optional pathogen model for users interested in simulating microbial pollution in a lake, reservoir, estuary or coastal environment. The model was developed based on *Cryptosporidium* sp. oocyst dynamics, and also contains variations for simulating indicator organisms such as coliform bacteria.

1.2.11 Metals For reservoir applications where metal release under anoxia is important, a simple model for iron, manganese and aluminium can be activated. This accounts for sediment release and conversion between particulate and dissolved forms.

1.3 Analysis Tools

Several useful analysis capabilities have been incorporated into CAEDYM to allow for greater utilization of the simulation output. Firstly, a time series location can be nominated by the user at a depth (DYRESM) or grid cell (ELCOM) where CAEDYM provides the values of all simulated process components and limitations for algal biology. Hence, the modeler can readily determine the dominant processes and rates at specified locations and its variability in time. This is exemplified later by evaluating the phytoplankton dynamics of two differing reservoirs. CAEDYM also allows the user to integrate all process rates and limitations over the entire water body. This feature enables the user to quantify major pools, sources and sinks.

Since CAEDYM v2.0, users may also choose to output numerous 'derived' variables. These are variables calculated for output only that provide more specific information of interest such as rates and other information rather than just looking at basic state variable concentrations.

Both the time-series files and derived output are discussed in more detail in the CAEDYM User Manual.

Light

2.1 Photosynthetically Active Radiation

Incident shortwave radiation supplied to the hydrodynamic driver for the surface thermodynamics model is passed to CAEDYM. For primary production, the shortwave intensity at the surface is converted to the photosynthetically active component (PAR; 400-700nm) by assuming it composes 45% of the incident spectrum (Jellison and Melack, 1993). It is assumed to penetrate into the water column according to Beer's Law:

$$I_{PAR_z} = 0.45I_0e^{\eta_{PAR}z} \quad (2.1)$$

where I_{PAR_z} is the photosynthetically active radiation at depth z m below the surface, I_0 is the incident shortwave intensity, and η_{PAR} is the PAR extinction coefficient. This varies spatially and temporally within the model according to the concentrations of algae, inorganic and detrital particles, and DOC:

$$\eta_{PAR} = \eta_w + \sum_a^{N_A} K_e^{A_a} A_a + \sum_d^{N_D} K_e^{DOC_d} DOC_d + \sum_d^{N_D} K_e^{POC_d} POC_d + \sum_s^{N_S} K_e^{SS_s} SS_s \quad (2.2)$$

where η_w is attenuation due to pure water (constant), and K_e is the rate the extinction coefficient increases with increasing concentration of the corresponding variable, as listed in the superscript ($g^{-1} m^3 m^{-1}$).

2.2 Ultraviolet Radiation

In addition to PAR, the photolytic decay of refractory DOC and microbial/pathogen inactivation also require the intensity of ultra-violet (UV) radiation throughout the water column. The UV incident at the water surface is predominantly within the UV-A band, which is approximately 3% of the incident solar radiation (Grant et al 1997). It decays throughout the water column similarly to (2.1):

$$I_{UV_z} = 0.03I_0e^{\eta_{UV}z} \quad (2.3)$$

where η_{UV} is the extinction coefficient for UV-A light. UV-B and UV-C bandwidths may also be activated within the code easily for more detailed investigations, but are not enabled in the public release executables.

Inorganic Particles

Two size classes of inorganic particles may be configured within CAEDYM using the state variables *SSOL1* and *SSOL2*. The user may specify different particle diameters, densities and critical shear stresses for the two groups. Note that although these groups are often termed ‘suspended solids’, CAEDYM treats these solely as the inorganic component of what may be routinely measured as suspended solids. If this is the case, the user must add the other particulate state variables (particulate detritus and phytoplankton for example) to the inorganic particle mass to get the total suspended solid concentration for comparison with the field data. For this reason, *SS₁* and *SS₂* are termed inorganic particles within this document to avoid confusion.

Inorganic particles within CAEDYM are simply modelled by accounting for settling and resuspension. Although they are involved in the adsorption and desorption of nutrients, the adsorbed (i.e. particulate inorganic) nutrients have their own state variables (*PIP* and *PIN*) and so do not impact on the *SS* masses directly (refer to Section 5). The equation for inorganic suspended solids is therefore:

$$\frac{\partial SS_s}{\partial t} = \underbrace{\frac{v_s}{\Delta z} SS_s}_{\text{settling}} + \underbrace{\alpha_{S_s} \frac{\tau - \tau_{c_s}}{\tau_{ref}} \frac{SS_{s-sed}}{K_{SS_s} + SS_{s-sed}} \frac{1}{\Delta z_{bot}}}_{\text{resuspension}} \quad (3.1)$$

where SS_s is the concentration of inorganic suspended solids for group s ($g\ m^{-3}$), v_s is the settling velocity ($m\ s^{-1}$), Δz is the grid or layer thickness, α_{S_s} is the resuspension rate parameter (discussed in some detail in Section 10.2) which has units of $g\ m^{-2}\ s^{-1}$, τ is the shear stress ($N\ m^{-2}$), τ_{c_s} is the critical shear stress for group s , τ_{ref} is a reference shear stress (usually set to $1\ N\ m^{-2}$), K_{SS_s} controls the effect of sediment limitation on resuspension (g), and SS_{s-sed} is the sediment *SS* mass of group s (g).

The settling velocity is calculated according to Stoke’s Law according to the user defined particle density, ρ_{S_s} , and diameter, d_{S_s} :

$$v_s = g \frac{(\rho_{S_s} - \rho_w) d_{S_s}^2}{18\mu} \quad (3.2)$$

where ρ_w is the density of water and μ is the dynamic viscosity of water calculated internally as a function of temperature.

Dissolved Oxygen

4.1 Introduction

The following processes are considered as part of the model for dissolved oxygen (DO) as shown schematically in Figure 4.1:

- a: exchange to and from the air/water interface (Section 4.2)
- b: utilisation of oxygen at the sediment/water interface (i.e. the sediment oxygen demand) (Section 4.3)
- c: utilisation of oxygen as bacteria degrade organic matter (i.e. the water column BOD) (Section 4.4)
- d: utilisation of oxygen in the process of nitrification (Section 4.5)
- e: photosynthetic oxygen production and respiratory consumption by phytoplankton (Section 4.6)
- f: utilisation of oxygen due to respiration by zooplankton (Section 4.7)
- g: photosynthetic oxygen production and respiratory consumption by macroalgae (Section 4.8)
- h: photosynthetic oxygen production and respiratory consumption by seagrasses/macrophytes (Section 4.9)
- i: utilisation of dissolved oxygen due to photosynthesis and respiration in jellyfish (Section 4.10)
- j: utilisation of dissolved oxygen due to respiration of higher organisms (macroinvertebrates, fish) (Section 4.11)

The rate equation for dissolved oxygen (DO) takes the form:

$$\frac{\partial DO}{\partial t} = \underbrace{f_{O_2}^{ATM}}_{\text{a-atm flux}} - \underbrace{f_{O_2}^{DSF}}_{\text{b-sed flux}} - \underbrace{f_{O_2}^{DEC}}_{\text{c-BOD}} - \underbrace{f_{O_2}^{NIT}}_{\text{d-nitrification}} + \underbrace{f_{O_2}^{PHY}}_{\text{e-phyto}} - \underbrace{f_{O_2}^{ZOO}}_{\text{f-zoop}} + \underbrace{f_{O_2}^{MAC}}_{\text{g-maca}} + \underbrace{f_{O_2}^{SEA}}_{\text{h-sea/mphyte}} - \underbrace{f_{O_2}^{JEL}}_{\text{i-jellies}} \quad (4.1)$$

and each of these functions are discussed in more detail below.

4.2 Atmospheric Exchange

Atmospheric exchange is based on the model of Wanninkhof (1992), where the flux of oxygen, F_{O_2} , across the air-water boundary ($gm^{-2}s^{-1}$) is given by:

$$F_{O_2} = k_{O_2} (C_{air} - C_{water}) \quad (4.2)$$

where k_{O_2} (ms^{-1}) is the oxygen transfer coefficient, C_{water} (gm^{-3}) is the oxygen concentration in the surface waters near the interface and C_{air} (gm^{-3}) is the concentration of oxygen in the air phase near the interface. A positive flux represents input of oxygen from the atmosphere to the water. C_{air} is dependent on temperature, T , salinity, S and atmospheric pressure, p , as given by Riley and Skirrow (1974):

$$C_{air}(T, S, p) = 1.42763 f(p) \exp \left\{ -173.4292 + 249.6339 \left[\frac{100}{\theta_k} \right] + 143.3483 \ln \left[\frac{\theta_k}{100} \right] - 21.8492 \left[\frac{\theta_k}{100} \right] + S \left(-0.033096 + 0.014259 \left[\frac{\theta_k}{100} \right] - 0.0017 \left[\frac{\theta_k}{100} \right]^2 \right) \right\} \quad (4.3)$$

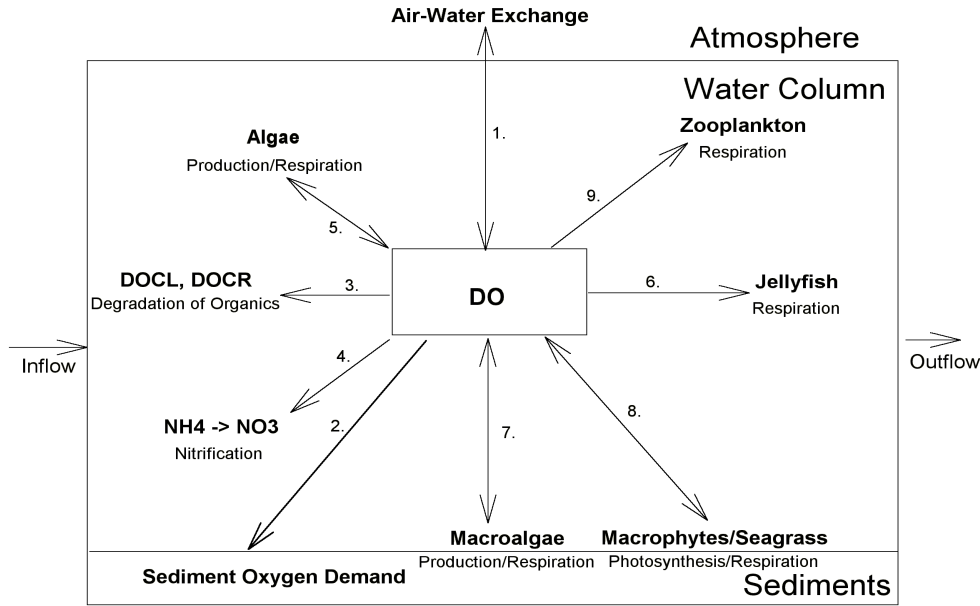


Figure 4.1 Simplified schematic of the dissolved oxygen (DO) dynamics within CAEDYM.

where θ_k is temperature in degrees Kelvin, salinity is expressed as parts per thousand and atmospheric pressure is in kPa . The pressure correction function, $f(p)$ varies between one and zero for the surface and high altitudes respectively:

$$f(p) = \frac{p_H}{p_{SL}} \left[1 - \frac{p_{vap}}{p_H} \right] / \left[1 - \frac{p_{vap}}{p_{SL}} \right]. \quad (4.4)$$

Here, p_H is the pressure at altitude H (kPa), p_{SL} is the sea level pressure ($101.32kPa$) and p_{vap} is the water vapour pressure in kPa . p_H is related to the altitude (m above sea level) specified in the input files following the familiar:

$$p_H = p_{SL} - \frac{\rho_{air}gH}{1000} \quad (4.5)$$

where ρ_{air} is the density of air and g is acceleration due to gravity.

The value of k_{O_2} (ms^{-1}) is given by (Wanninkhof, 1992):

$$k_{O_2} = 11.16u^2 \left[\frac{Sc}{660} \right]^{-0.5}, \quad (4.6)$$

where u is the wind speed 10m above the surface and Sc is the Schmidt number determined by:

$$Sc = \left(0.9 + 0.1 \frac{S}{350} \right) [1953.4 - 128.0T + 3.9918T^2 - 0.05009T^3]. \quad (4.7)$$

where T is water temperature in degrees celsius. In the above expression a linear dependence is assumed between the Schimdt Number and salinity as only fresh and saltwater temperature-dependent equations are given by Wanninkhof (1992).

The final oxygen function in units of $g\ m^{-3}\ day^{-1}$ (only applicable to the surface layer of depth z_{surf}), is therefore defined according to:

$$f_{O_2}^{ATM} = \frac{86400 F_{O_2}}{z_{surf}}. \quad (4.8)$$

4.3 Sediment Oxygen Consumption

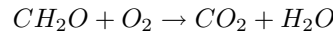
A simple sediment oxygen flux model is currently employed within CAEDYM and operates by assuming the flux is simply a function of the overlying water temperature and dissolved oxygen concentration (i.e a ‘static’ model). The change in concentration of dissolved oxygen in the layer immediately above the sediments is given by:

$$f_{O_2}^{DSF}(T, DO, 0) = S_{SOD} f_{SOD}^{T2}(T) f_{SOD}^{DO1}(DO) \quad (4.9)$$

where S_{SOD} is a fixed oxygen flux across the sediment-water interface and $K_{DO_{SOD}}$ is a half-saturation constant for the sediment oxygen demand. The assumptions under which this model is constructed may be considered broad, but ultimately the models performance dictates its usefulness. A more dynamic model for the sediment oxygen flux is currently under development and is expected for later releases.

4.4 Oxygen Consumption Through Microbial Decomposition of Organic Material

Microbial activity facilitates the breakdown of organic carbon (in particular, DOC) to CO_2 . This is an oxygen consuming process:



Therefore, for each carbon that is mineralized, a stoichiometrically equivalent amount of oxygen is removed:

$$f_{O_2}^{DEC}(T, DO, B^*, DOC) = \sum_d^{N_D} f_B^{T1}(T) \mu_{DEC_d} \min(f_B^{DOB}(DO), f_B^{BAC}(B)^*) DOC_d Y_{O_2:C} \quad (4.10)$$

where again $Y_{O_2:C}$ is the conversion of carbon to dissolved oxygen, and μ_{DEC} is the optimal mineralization rate of DOC when it is not limited by the amount of bacteria, B , DO or temperature, T . More detail on this process is described in Section 5.3.

4.5 Oxygen Utilisation in the Process of Nitrification

The process of nitrification requires oxygen as modelled by:

$$f_{O_2}^{NIT} = \mu_{NIT} f_{NIT}^{T2}(T) f_{NIT}^{DO1}(DO) NH_4 Y_{NH} \quad (4.11)$$

where Y_{NH} is a stoichiometric factor for the ratio of oxygen to nitrogen in the nitrification process, NH_4 is the ammonium concentration, μ_{NIT} is the nitrification rate coefficient (day^{-1}) and $K_{DO_{NIT}}$ is a half-saturation constant for the effect of oxygen limitation on the nitrification process.

4.6 Oxygen Production and Utilisation by Phytoplankton

Photosynthetic oxygen production and respiratory oxygen utilisation by phytoplankton is given by the following equation, which sums over the number of simulated phytoplankton groups, $nphy$:

$$f_{O_2}^{PHY} = \sum_{a=1}^{N_A} \{ (\mu_{MAX_a} \min[f(I)_a, f(N)_a, f(P)_a, f(Si)_a^*, f(C)_a^{**}] f_{A_a}^{T1}(T)) (1 - k_p) - R_a f(S)_a \} Y_{O_2:C} Y_{C:Chla} A_a \quad (4.12)$$

where, μ_{MAX_a} is the maximum growth rate of group a (day^{-1}), A_a is the concentration of the a^{th} algal group ($g\ Chla\ m^{-3}$), k_p is the rate of photorespiration (day^{-1}), and R_a is respiration/metabolic loss rate (day^{-1}). The final two conversion factors, $Y_{O_2:C}$ and $Y_{C:Chla}$, are stoichiometric factors that convert chlorophyll-a to carbon, and carbon to dissolved oxygen (if phytoplankton are being simulated in carbon units then the latter conversion is not included). This equation is discussed in some detail during the description of the phytoplankton model (Section 6.2).

4.7 Oxygen Consumption by Zooplankton

Respiration by zooplankton consumes oxygen as is given by the following equation, which sums over the number of simulated zooplankton groups, $nzoo$:

$$f_{O_2}^{ZOO} = \sum_z^{N_Z} [k_{r_{Zz}} Z_z] Y_{O_2:C} \quad (4.13)$$

where, $k_{r_{Zz}}$ is the respiration rate of group z (day^{-1}), Z_z is the concentration of the z^{th} zooplankton group ($g\ C\ m^{-3}$), and $Y_{O_2:C}$ is the stoichiometric factor for carbon to dissolved oxygen. More detail on the zooplankton model is provided in Section 6.3.

4.8 Oxygen Production and Utilisation by Macroalgae

Photosynthetic oxygen production and respiratory oxygen utilisation by macroalgae is given by the following equation, which sums over the number of simulated macroalgae groups, N_M :

$$f_{O_2}^{MAC} = \sum_m^{N_M} [(\mu_{MAX_m} \min[f(I)_m, f(N)_m, f(P)_m] f_{M_m}^{T1}(T)) - R_m f(S)_m] Y_{O_2:C} M_m / h_{mac} \quad (4.14)$$

where, μ_{MAX_m} is the maximum growth rate of group m (day^{-1}), M_m is the macroalgal concentration for the m^{th} group ($g\ C\ m^{-2}$), h_{mac} is the height of the benthic macroalgal bed (in m), and R_m is respiration/metabolic loss rate (day^{-1}). The final conversion factor, $Y_{O_2:C}$ is the stoichiometric conversion between carbon and dissolved oxygen. This equation is discussed in some detail during the description of the macroalgae model (Section 7.2).

4.9 Oxygen Production and Consumption by Seagrasses/Macrophytes

Photosynthetic oxygen production and respiratory oxygen utilisation by seagrasses/macrophytes is given by the following equation, which sums over the number of simulated seagrass/macrophyte groups, n_{sea} :

$$f_{O_2}^{SEA} = \sum_m^{n_{sea}} \frac{(1 - f_{seaO_2}) k_{O:C} (\Delta B_m / \Delta t)}{z_{bot}} \quad (4.15)$$

where, f_{seaO_2} is the fraction of oxygen production that is imparted to the sediments as opposed to the water column, $\Delta B_m / \Delta t$ is the rate of change of biomass for the m^{th} group ($g C m^{-2} day^{-1}$), z_{bot} is the depth of the bottom layer (m), and $k_{O:C}$ is a conversion factor for seagrass/macrophyte biomass change to comparable O_2 production ($g O_2 (g C)^{-1}$). This equation is discussed in some detail during the description of the seagrass/macrophyte model (Section 7.3).

4.10 Oxygen Production and Utilisation by Jellyfish

The effect of jellyfish production of oxygen (via symbiotic algal cells) and respiration of oxygen is represented by an equation similar to the jellyfish production equation, but with slight modification to remove the consumption of organic matter by the jellyfish, which is accounted for in the POC term, and with inclusion of a yield term to convert jellyfish biomass changes to equivalent oxygen:

$$f_{O_2}^{JEL} = f_J(T) [GJ_{max} f(S) f(I) - k_{r,J}] J Y_{O:J} \quad (4.16)$$

Here, J is the jellyfish biomass as $mL medusae m^{-3}$, $Y_{O:J}$ converts the net jellyfish production to an equivalent oxygen yield, $k_{r,J}$ is the jellyfish respiration coefficient (day^{-1}), GJ_{max} is the maximum relative growth rate (day^{-1}), $f(S)$, $f(T)$ and $f(I)$ are factors that regulate the response to salinity, temperature and light respectively, as described in section 6.5.

4.11 Oxygen Utilisation by Higher Organisms

Utilisation of dissolved oxygen due to respiration of the remaining state variables represented in the model (e.g. bivalves, crustaceans and fish) is not considered to have a substantial influence on dissolved oxygen concentrations in most systems and so is assumed to be negligible.

Elemental Cycles and Balance Equations

5.1 Introduction

Elemental nutrients cycles of the dominant macronutrients of aquatic plants (phytoplankton, macrophytes and macroalgae) and animals (zooplankton, fish) have been incorporated into CAEDYM. Both the inorganic and organic forms of carbon, nitrogen, phosphorus, and silica are modeled explicitly. Further, CAEDYM explicitly simulates organic nutrients in both the filterable and particulate pools, and the labile and refractory components can optionally be resolved (set: $\text{reff} = \text{T}$). Though inorganic nutrients are modelled only as filterable, there is the provision for adsorption-desorption onto inorganic suspended solids. Atmospheric gas exchange between dissolved carbon dioxide and the atmosphere are also explicitly modeled by CAEDYM.

To take advantage of the similarity between the various biogeochemical cycles, a series of generic parameterizations are employed and described next.

5.2 Generic Parameterizations and Organic Matter Configuration

Table 5.1 provides the general equation forms of the simplest formulations used to model the:

1. temperature and oxygen dependencies (Eqs. 5.1-5.4)
2. dissolved sediment fluxes (Eq. 5.5)
3. atmospheric gas exchange (Eq. 5.6)
4. particle resuspension (Eq. 5.7)
5. particle settling (Eq. 5.8)
6. decomposition of organic matter (equation 5.9)
7. adsorption/desorption of dissolved inorganics to inorganic particles (Eq. 5.12)
8. mortality and excretion from aquatic flora and fauna (Eq. 5.13)
9. autotrophic uptake of dissolved inorganic nutrients (Eq. 5.14).
10. respiration by algae, macroalgae, zooplankton, fish and bacteria (Eq. 5.15).
11. grazing by zooplankton and fish (Eq. 5.16)

A schematic representation of a simple generic configuration of CAEDYM is provided in Figure 5.1. CAEDYM provides the flexibility to model the organic carbon, nitrogen, and phosphorus with different parameters as outlined throughout this chapter. One manner to reduce the number of parameters is to link transformation rates of each of these elements (organic carbon, nitrogen, phosphorus) into the same parameter for organic matter rates. In other words, decomposition (particulate to dissolved organics), mineralization (dissolved organics to dissolved inorganics),

Table 5.1 Generic parameterizations of processes used throughout the nutrient cycles of CAEDYM. The symbol g is used as a generic group identifier.

Temperature:

$$f_g^{T1}(T) = \vartheta_g^{T-20} + \vartheta_g^{k_g(T-a_g)} + b_g \quad (5.1)$$

$$f_g^{T2}(T) = \vartheta_g^{T-20} \quad (5.2)$$

Dissolved Oxygen:

$$f_g^{DO1}(DO) = \frac{DO}{K_{DO_g} + DO} \quad (5.3)$$

$$f_g^{DO2}(DO) = \frac{K_{DO_g}}{K_{DO_g} + DO} \quad (5.4)$$

Dissolved Sediment Flux:

$$f_g^{DSF}(T, DO, pH) = f_{SED}^{T2}(T) S_g \left(\frac{K_{DOS-g}}{K_{DOS-g} + DO} + \frac{|pH - 7|}{K_{pHS-g} + |pH - 7|} \right) \frac{1}{\Delta z_{bot}} \quad (5.5)$$

Atmospheric Gas Exchange:

$$f_g^{ATM}(g) = k_g (g^{atm} - g^{surf}) \quad (5.6)$$

Resuspension:

$$f_g^{RES}(g_{sed}) = \alpha_g (\tau - \tau_{cg}) \left(\frac{g_{sed}}{K_{sed-g} + g_{sed}} \right) \quad (5.7)$$

Settling:

$$f_g^{SET}(g) = \frac{v_g}{\Delta z} g \quad (5.8)$$

Decomposition of Organic Matter:

$$f_g^{DEC}(T, DO, B^*, g) = \left[\mu_{DEC_g} f_B^{T1}(T) \min \left(f_B^{DOB}(DO), f_B^{BAC}(B^*) \right) \right] g \quad (5.9)$$

where

$$f_B^{BAC}(B) = \frac{B}{K_B + B} \quad (5.10)$$

$$f_B^{DOB}(DO) = f_B^{DO1}(DO) + f_{AnB} f^{DO2}(DO) \quad (5.11)$$

Adsorption/Desorption:

$$f_g^{ADD}(SS1, SS2, g, y) = \frac{SS1 + SS2}{\rho_{SS}} (g k_{ad-g} - E0C_g) - y \quad (5.12)$$

Biological Mortality & Excretion:

$$f_g^{BME}(A, M, Z, F, B) = \underbrace{\sum_a^{N_A} E_g(A_a)}_{\text{a-phytoplankton}} + \underbrace{\sum_m^{N_M} E_g(M_m)}_{\text{b-macroalgae}} + \underbrace{\sum_z^{N_Z} E_g(Z_z)}_{\text{c-zooplankton}} + \underbrace{\sum_f^{N_F} E_g(F_f)}_{\text{d-fish}} + \underbrace{E_g(B)}_{\text{e-bacteria}} \quad (5.13)$$

Biological Uptake:

$$f_g^{BUP}(A, M, B, g) = \underbrace{\sum_a^{N_A} U_g(A_a)}_{\text{a-phytoplankton}} + \underbrace{\sum_m^{N_M} U_g(M_m)}_{\text{b-macroalgae}} + \underbrace{U_g(B)}_{\text{c-bacterial}} \quad (5.14)$$

Biological Respiration:

$$f_{DIC}^{BRE}(A, M, Z, F, B) = \underbrace{\sum_a^{N_A} R_{DIC}(A_a)}_{\text{a-phytoplankton}} + \underbrace{\sum_m^{N_M} R_{DIC}(M_m)}_{\text{b-macroalgae}} + \underbrace{\sum_z^{N_Z} R_{DIC}(Z_z)}_{\text{c-zooplankton}} + \underbrace{\sum_f^{N_F} R_{DIC}(F_f)}_{\text{d-fish}} + \underbrace{R_{DIC}(BAC)}_{\text{e-bacteria}} \quad (5.15)$$

Grazing:

$$f_g^{GRZX}(Z, F, g) = \underbrace{\sum_z^{N_Z} G_X(Z_z) f_g^{ZGW}(g)}_{\text{a-zooplankton}} + \underbrace{\sum_f^{N_F} G_X(F_f) f_g^{FGW}(g)}_{\text{b-fish}} \quad (5.16)$$

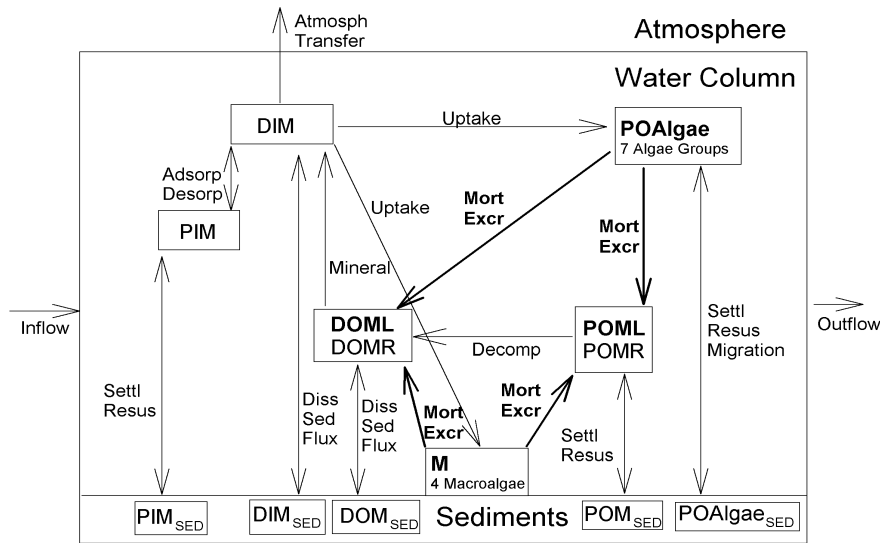


Figure 5.1 Generic schematic of the nutrient dynamics with CAEDYM.

and settling (particle closure) rates would all be given the same parameter values, and all variables (particulate organic carbon, nitrogen, and phosphorus) considered one particle for these processes (Romero et al., 2003).

The oxygen and temperature dependencies, f^{DO} and f^T , are common in the decomposition and mineralisation functions for C , N and P . The oxygen dependence allows for enhanced breakdown in high oxygen and some ability under anoxia, i.e. microbial decomposition of organics is assumed to be primarily mediated by facultative heterotrophs. Here f_{AnB} is the efficiency of microbial activity when under complete anoxia, and K_{DOB} is the half-saturation constant for the dependence of oxygen on detrital breakdown. The temperature function for microbial decomposers is identical to that for algae and other biological groups, f^{T1} (see Section 6.2).

The other functions for mortality/excretion, E_g , uptake, U_g and respiration, R_g are defined in detail in Chapters 6 and 7 for the respective biological groups.

5.3 Carbon

Carbon is considered the primary 'currency' within CAEDYM v2, and the carbon cycle forms the backbone upon which the other elemental cycles are based. Although it is still common for most applications to use chlorophyll-a as the units of the phytoplankton species, carbon is still the basic unit and the equations presented reflect this. If the reader is using chlorophyll-a for phytoplankton (as chosen using the 'CorChla' flag in the configuration file), then it is important to bear in mind the chlorophyll-a to carbon ratio, $Y_{C:Chla}$, for the phytoplankton balance equation. For more information on this refer to the phytoplankton chapter (6.2).

At least 3 (if only one algal group and up to 9 with 7 algal groups) mandatory and numerous optional (refractory

Table 5.2 Carbon state variables simulated by CAEDYM. Modelled mechanisms for each state variable are provided. Macroalgae and all other biotic state variables have internal stores of C tracked. Sediment state variables mass balance is maintained with interactions with the water column, however no sediment transformations occur.

Variable	Name	Process Description
Mandatory State Variables:		
DOCL	Labile Dissolved Organic Carbon	Equation 5.18: <i>Mineralization, decomposition of POCL, algal mortality/excretion, sediment flux, zooplankton fluxes, photolytic decay of DOCL</i>
POCL	Labile Particulate Organic Carbon	Equation 5.20: <i>Microbial decomposition to DOCL, settling, resuspension, algal mortality/excretion, zooplankton fluxes, macroinvertebrate fluxes</i>
A	Algal Internal Carbon (1 compulsory, upto 7 available)	Equation 5.23: <i>Algal uptake (photosynthesis) and respiration, settling, resuspension, algal excretion/mortality, zooplankton & fish grazing, bivalve grazing</i>
Optional State Variables:		
DOCR	Refractory Dissolved Organic Carbon	Equation 5.19: <i>Mineralization, decomposition of POCL, sediment flux, photolytic decay</i>
POCR	Refractory Particulate Organic Carbon	Equation 5.21: <i>Decomposition to DOCL, settling, resuspension, polychaete consumption</i>
DIC	Dissolved Inorganic Carbon	Equation 5.17: <i>Algal uptake (photosynthesis), mineralization of DOC, sediment flux, seagrass/macrophyte metabolism, atmospheric exchange of CO₂, zooplankton respiration</i>
B	Bacterial Biomass	Equation 5.22: <i>Consumption & excretion of DOC, respiration, settling, resuspension, zooplankton & fish grazing</i>
Z	Zooplankton Biomass (0 compulsory groups, upto 5 available)	Equation 5.24: <i>Grazing, excretion, mortality, predation</i>
F	Fish Biomass (0 compulsory groups, upto 3 available)	Equation 5.25: <i>Grazing, excretion, mortality, predation</i>

organics, dissolved inorganic, and higher biology) carbon state variables are tracked by CAEDYM (Table 5.2). A schematic process representation (Figure 5.2) illustrates that the sources of the labile forms include fresh senescent organic material, whereas the refractory do not have these sources. The governing partial differential equations of all the processes of carbon fate in the sediments and water column are summarized in Table 5.3.

The main processes involved in carbon fate in the sediments and water column are:

1. Atmospheric fluxes of *DIC*.
2. Carbonate buffer system induced *DIC* variations.
3. Mineralization of *DOCL* and *DOCR* to *DIC*.
4. Biological uptake of *DIC* by phytoplankton, macroalgae and macrophytes into the *IC* pool.
5. Dissolved sediment fluxes of *DIC*, *DOCL*, and *DOCR*.
6. Decomposition of *POCL* to *DOCL* and *POCR* to *DOCR*.
7. Biological mortality and excretion into the *DOCL* and *POCL* pools.
8. Settling of *POCL*, *POCR* and *IC*.

Table 5.3 CAEDYM carbon cycle. All state variables also have source of inflows and loss via outflows and are subject to advection and mixing by the hydrodynamic driver.

$$\begin{aligned} \frac{\partial DIC}{\partial t} = & \underbrace{f_{DOCL}^{MIN}(T, DO, DOCL)}_{\text{a-labile DOC minrzn (if bacf=F)}} + \underbrace{f_{DOCR}^{MIN}(T, DO, DOCR)}_{\text{b-refrac DOC minrzn (if bacf=F)}} + \underbrace{f_{DIC}^{DSF}(T, DO, pH)}_{\text{c-sediment flux}} + \\ & - \underbrace{f_{DIC}^{BUP}(A, M, DIC)}_{\text{d-biological uptake}} + \underbrace{f_{DIC}^{BRE}(A, M, Z, F, B)}_{\text{e-biological respiration}} + \underbrace{f_{DIC}^{ATM}(pCO_2)}_{\text{f-atmos flux}} \end{aligned} \quad (5.17)$$

$$\begin{aligned} \frac{\partial DOCL}{\partial t} = & \underbrace{f_{POCL}^{DEC}(T, DO, B^*, POCL)}_{\text{a-POCL decomposition}} - \underbrace{f_{DOCL}^{MIN}(T, DO, DOCL)}_{\text{b-DOCL mineralization}} \\ & + \underbrace{f_{DOCL}^{DSF}(T, DO, pH)}_{\text{c-sediment flux}} + \underbrace{f_{DOCL}^{BME}(A, M, Z, F, B)}_{\text{d-biological mort/excr}} + \underbrace{f_{DOCR}^{PLD}(DOCR, UV)}_{\text{e-photolytic decay}} \end{aligned} \quad (5.18)$$

$$\begin{aligned} \frac{\partial DOCR}{\partial t} = & \underbrace{f_{POCR}^{DEC}(T, DO, B^*, POCR)}_{\text{a-POCR decomposition}} - \underbrace{f_{DOCR}^{MIN}(T, DO, DOCR)}_{\text{b-DOCR mineralization}} \\ & + \underbrace{f_{DOCR}^{DSF}(T, DO, pH)}_{\text{c-sediment flux}} - \underbrace{f_{DOCR}^{PLD}(DOCR, UV)}_{\text{d-photolytic decay}} \end{aligned} \quad (5.19)$$

$$\begin{aligned} \frac{\partial POCL}{\partial t} = & - \underbrace{f_{POCL}^{DEC}(T, DO, B^*, POCL)}_{\text{a-POCL decomposition}} + \underbrace{f_{POCL}^{SET}(POCL)}_{\text{b-settling}} + \underbrace{f_{POCL}^{RES}(POCL_{sed})}_{\text{c-resuspension}} \\ & + \underbrace{f_{POCL}^{BME}(A, M, Z, F)}_{\text{d-biological mort/excr}} + \underbrace{\sum_z k_{mfz} G_C(Z_z)}_{\text{e-zoop messy feeding}} + \underbrace{\sum_f k_{mf_f} G_C(F_f)}_{\text{f-fish messy feeding}} \end{aligned} \quad (5.20)$$

$$\frac{\partial POCR}{\partial t} = - \underbrace{f_{POCR}^{DEC}(T, DO, B^*, POCR)}_{\text{a-POCR decomposition}} + \underbrace{f_{POCR}^{SET}(POCR)}_{\text{b-settling}} + \underbrace{f_{POCR}^{RES}(POCR_{sed})}_{\text{c-resuspension}} \quad (5.21)$$

$$\begin{aligned} \frac{\partial B}{\partial t} = & \underbrace{U_{DOCL}(B)}_{\text{a-uptake}} + \underbrace{U_{DOCR}(B)}_{\text{a-uptake}} - \underbrace{E_{DOCL}(B)}_{\text{b-excretion}} - \underbrace{R_{DIC}(B)}_{\text{c-respiration}} + \underbrace{f_B^{SET}(B)}_{\text{d-settling}} + \underbrace{f_B^{RES}(B_{sed})}_{\text{e-resuspension}} \\ & - \underbrace{f_B^{GRZC}(Z, F, B)}_{\text{e-grazing}} \end{aligned} \quad (5.22)$$

$$\begin{aligned} \frac{\partial A_a}{\partial t} = & \underbrace{U_{DIC}(A_a)}_{\text{a-uptake}} - \underbrace{E_{DOCL}(A_a)}_{\text{b-mortality \& excretion}} - \underbrace{E_{POCL}(A_a)}_{\text{b-mortality \& excretion}} - \underbrace{R_{DIC}(A_a)}_{\text{c-respiration}} \\ & + \underbrace{f_{A_a}^{SET}(A_a)}_{\text{d-settling}} + \underbrace{f_{A_a}^{RES}(A_{sed})}_{\text{e-resuspension}} - \underbrace{f_{A_a}^{GRZC}(Z, F, A_a)}_{\text{f-grazing}} \end{aligned} \quad (5.23)$$

$$\frac{\partial Z_z}{\partial t} = \underbrace{(1 - k_{mfz}) G_C(Z_z)}_{\text{a-grazing}} - \underbrace{E_{DOCL}(Z_z) - E_{POCL}(Z_z)}_{\text{b-excretion \& mortality}} - \underbrace{f_{Z_z}^{GRZC}(Z, F, Z_z)}_{\text{c-predation}} \quad (5.24)$$

$$\frac{\partial F_f}{\partial t} = \underbrace{(1 - k_{mf_f}) G_C(F_f)}_{\text{a-grazing}} - \underbrace{E_{DOCL}(F_f) - E_{POCL}(F_f)}_{\text{b-excretion \& mortality}} - \underbrace{f_{F_f}^{GRZC}(0, F, F_f)}_{\text{c-predation}} \quad (5.25)$$

$$TOC = DOCL + DOCR + POCL + POCR + B + \sum_a^{N_A} A_a + \sum_z^{N_Z} Z_z \quad (5.26)$$

$$TPOC = POCL + POCR + B + \sum_a^{N_A} A_a + \sum_z^{N_Z} Z_z \quad (5.27)$$

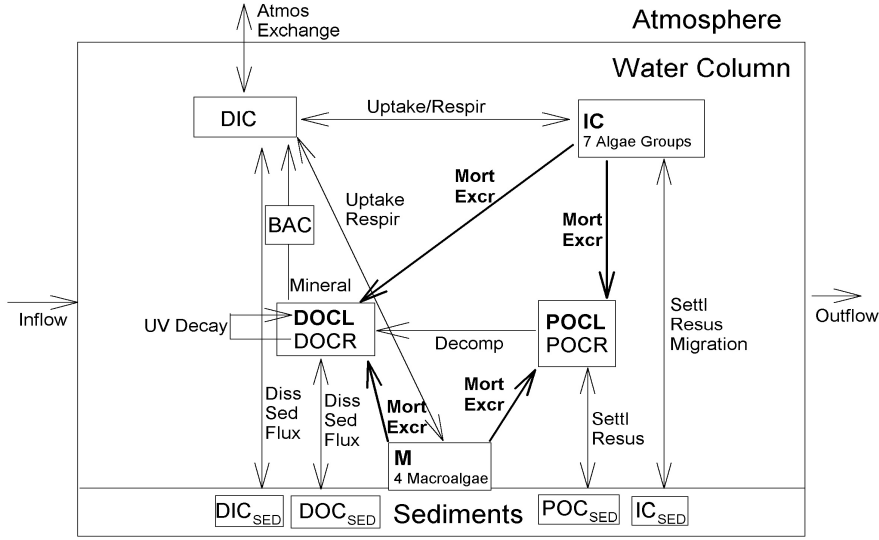


Figure 5.2 Simplified schematic of the carbon dynamics with CAEDYM.

9. Resuspension of $POCL$, $POCR$ and IC .

5.3.1 Dissolved Inorganic Carbon - Atmospheric Fluxes: Carbon dioxide (CO_2) transfer across the air-water interface, F_{CO_2} ($gm^{-2}s^{-1}$), is calculated following (Wanninkhof, 1992):

$$F_{CO_2} = k_{CO_2} K_0 (pCO_2^{water} - pCO_2^{air}) \quad (5.28)$$

where pCO_2 is the partial pressure of CO_2 (atm), k_{CO_2} is the gas transfer velocity (ms^{-1}), calculated as:

$$k_{CO_2} = 2.2 \times 10^{-5} \frac{u_{10}^2}{\sqrt{Sc}} \quad (5.29)$$

where u_{10} is the wind speed 10m above the surface and Sc is the Schmidt number, defined as:

$$Sc = \left(0.9 + \frac{S}{350}\right) [2073.1 - 125.62T + 3.6276T^2 - 0.043219T^3] \quad (5.30)$$

Here, S is the salinity of water (psu) and T is the water temperature in degrees Celcius. The solubility product of carbon dioxide, K_0 ($molL^{-1}atm^{-1}$) is calculated according to (Weiss, 1974):

$$K_0 = \exp(-58.0931 + 90.5069 \left[\frac{100}{\theta_K}\right] + 22.294 \ln \left[\frac{\theta_K}{100}\right] + 0.027766S - 0025888S \left[\frac{\theta_K}{100}\right] + 0.0050578S \left[\frac{\theta_K}{100}\right]^2), \quad (5.31)$$

where θ_K is the water temperature in degrees Kelvin.

Finally, the atmospheric flux function in equation 5.17 is defined as:

$$f_{DIC}^{ATM} = 2.63 \times 10^4 \frac{F_{CO_2}}{z_{surf}}, \quad (5.32)$$

where z_{surf} is the depth of the grid/layer closest to the surface (m) as the atmospheric exchange only operates in the surface layer immediately adjacent to the atmosphere. The constant is used to convert the mass of CO_2 into equivalent C , and to convert seconds to days.

5.3.2 Dissolved Inorganic Carbon - Carbonate Kinetics: The non-equilibrium carbonate kinetics are modelled using the approach of Butler (1982). The water column is modelled as a closed system, as in a titration, where fluxes into and out of the system are specified, such as fluxes due to inflows, or atmospheric exchange. In a closed carbonate system, the total alkalinity (TA), dissolved inorganic carbon concentration (DIC) and pH are related by (Butler, 1982),

$$TA = DIC \frac{K_{a1}[H^+] + 2K_{a1}K_{a2}}{[H^+]^2 + K_{a1}[H^+] + K_{a1}K_{a2}} + \frac{K_w}{[H^+]} - [H^+] \quad (5.33)$$

where K_w is the ion product of water, K_{a1} is the first acidity constant, K_{a2} is the second acidity constant. pH is calculated from:

$$pH = -\log_{10}[H^+] \quad (5.34)$$

and DIC is defined as:

$$DIC = [CO_3^{2-}] + [HCO_3^-] + [CO_2] + [H_2CO_3] \quad (5.35)$$

where all concentrations are in ($molL^{-1}$). Note that the concentration of hydrated carbon dioxide, $[H_2CO_3]$, is considered to be negligible and is therefore omitted.

The conversion between the carbon dioxide partial pressure, pCO_2 and carbon dioxide concentration ($molL^{-1}$) is given by:

$$[CO_2] = K_H pCO_2 \quad (5.36)$$

where K_H is the activity coefficient.

The ionic strength of the water impacts the dissociation constants. Ionic strength, I , is typically defined as (Butler, 1982):

$$I = 0.5 ([Na^+] + [H^+] + [HCO_3^-] + 4[CO_3^{2-}] + [H^+]/K_w). \quad (5.37)$$

Rather than model this explicitly, the ionic strength is entered into the model as a constant, and is not assumed to vary significantly in space or time for a given system. From the ionic strength, an activity coefficient is defined as:

$$f = \left(\frac{I^{1/2}}{1 + I^{1/2}} - 0.2I \right) \left(\frac{298}{\theta_C + 273} \right)^{2/3}. \quad (5.38)$$

The dissociation constants are then computed following:

$$\log_{10} (K_H^{i+1}) = \log_{10} (K_H^0) - bI \quad (5.39)$$

$$\log_{10} (K_w^{i+1}) = \log_{10} (K_w^0) + f \quad (5.40)$$

$$\log_{10} (K_{a1}^{i+1}) = \log_{10} (K_{a1}^0) + f + bI \quad (5.41)$$

$$\log_{10} (K_{a2}^{i+1}) = \log_{10} (K_{a2}^0) + 2f \quad (5.42)$$

where $b = 0.105$ (Butler, 1982).

For this system, if two of the three components (i.e. TA , pH or DIC) are known the third can be determined. Therefore, within CAEDYM, pH and DIC are tracked as state variables, although for those interested, at each time step TA is also computed and output via the time series files.

The carbonate speciation for a given value of pH and DIC is then estimated from:

$$[CO_3^{2-}] = DIC \frac{K_{a1}K_{a2}}{[H^+]^2 + K_{a1}[H^+] + K_{a1}K_{a2}}, \quad (5.43)$$

$$[HCO_3^-] = DIC \frac{K_{a1}[H^+]}{[H^+]^2 + K_{a1}[H^+] + K_{a1}K_{a2}}, \quad (5.44)$$

$$[CO_2] = DIC \frac{[H^+]^2}{[H^+]^2 + K_{a1}[H^+] + K_{a1}K_{a2}}. \quad (5.45)$$

Using this framework, the inorganic carbon model within CAEDYM operates as follows:

1. from initial field measurements of TA and pH , calculate DIC using 5.33
2. calculate initial carbonate speciation using 5.43-5.45
3. calculate partial pressure of CO_2 using 5.36
4. start timestep loop
5. calculate atmospheric CO_2 flux using 5.32
6. calculate internal CO_2 fluxes from phytoplankton photosynthesis/respiration, zooplankton respiration and bacterial respiration
7. calculate new DIC using 5.35
8. assuming TA constant, as CO_2 does not change the alkalinity directly, calculate new pH by iteratively solving 5.33
9. calculate new carbonate speciation using 5.43-5.45
10. calculate new partial pressure of CO_2 using 5.36
11. update new TA and DIC

Table 5.4 Phosphorus state variables simulated by CAEDYM. Modelled mechanisms for each state variable are provided. Macroalgae and all other biotic state variables have internal stores of P tracked. Sediment state variables mass balance is maintained with interactions with the water column, however no sediment transformations occur.

Variable	Name	Process Description
Mandatory State Variables:		
FRP	Filterable Reactive Phosphorus	Equation 5.47: <i>Autotrophic uptake, mineralization, sediment flux, adsorption/desorption</i>
DOPL	Labile Dissolved Organic Phosphorus	Equation 5.47: <i>Mineralization, decomposition of POPL, algal mortality/excretion, sediment flux, zooplankton & fish contribution</i>
POPL	Labile Particulate Organic Phosphorus	Equation 5.49: <i>Decomposition to DOPL, settling, algal mortality/excretion, resuspension, zooplankton & fish fluxes</i>
AIP	Algal Internal Phosphorus (1 compulsory group, upto 7 available)	Equation 5.53: <i>Algal uptake, settling, resuspension, algal excretion/mortality, zooplankton & fish grazing</i>
Optional State Variables:		
DOPR	Refractory Dissolved Organic Phosphorus	Equation 5.48: <i>Mineralization, decomposition of POPR, sediment flux</i>
POPR	Refractory Particulate Organic Phosphorus	Equation 5.50: <i>Decomposition to DOPR, settling, resuspension</i>
PIP	Particulate Inorganic Phosphorus	Equation 5.51: <i>Adsorption/desorption, settling, resuspension</i>
BIP	Bacterial Internal Phosphorus	Equation 5.52: <i>Uptake, excretion, settling, resuspension, grazing</i>
ZIP	Zooplankton Internal Phosphorus (0 compulsory groups, upto 5 available)	Equation 5.54: <i>Grazing, excretion, mortality, predation</i>
FIP	Fish Internal Phosphorus (0 compulsory groups, upto 3 available)	Equation 5.55: <i>Grazing, excretion, mortality, predation</i>

5.4 Phosphorus

At least four (if only one algal group and up to 10 with 7 algal groups) mandatory and numerous optional (refractory organics, particulate inorganic and higher biology) phosphorus state variables can be simulated by CAEDYM (Table 5.4). A schematic process representation (Figure 5.3) illustrates that the sources of the labile forms include fresh senescent organic material, whereas the refractory do not. The governing balance equations for all simulatable phosphorus variables showing all the processes in the sediments and water column are summarized in Table 5.5.

The main processes involved in phosphorus transformations in the sediments and water column are:

1. Mineralization of *DOPL* and *DOPR* to *FRP* (directly or through bacteria).
2. Biological uptake of *FRP* by phytoplankton and macroalgae into the internal pools.
3. Dissolved sediment fluxes of *FRP*, *DOPL*, and *DOPR*.
4. Adsorption/desorption of PO_4 onto inorganic suspended solids into *PIP* pool.
5. Decomposition of *POPL* to *DOPL* and *POPR* to *DOPR*.

Table 5.5 CAEDYM phosphorus cycle mass balance equations. All state variables also have source of inflows and loss via outflows and are subject to advection and mixing by the hydrodynamic driver.

$$\frac{\partial FRP}{\partial t} = \underbrace{f_{DOPL}^{MIN}(T, DO, DOPL)}_{\text{a-labile DOP minrzn (if bacf=F)}} + \underbrace{f_{DOPR}^{MIN}(T, DO, DOPR)}_{\text{b-refrac DOP minrzn (if bacf=F)}} + \underbrace{f_{FRP}^{BME}(0, 0, 0, 0, B^*)}_{\text{c-bacterial minrzn (if bacf=T)}} \quad (5.46)$$

$$- \underbrace{f_{FRP}^{BUP}(A, M, B, FRP)}_{\text{d-biological uptake}} + \underbrace{f_{FRP}^{DSF}(T, DO, pH)}_{\text{e-sediment flux}} + \underbrace{f_{FRP,PIP}^{ADD}(SS1, SS2, PO_4, PIP)}_{\text{f-adsorption/desorption}}$$

$$\begin{aligned} \frac{\partial DOPL}{\partial t} = & \underbrace{f_{POPL}^{DEC}(T, DO, POPL)}_{\text{a-POPL decomposition}} - \underbrace{f_{DOPL}^{MIN}(T, DO, B^*, DOPL)}_{\text{b-DOPL mineralization}} + \underbrace{f_{DOPL}^{DSF}(T, DO, pH)}_{\text{c-sediment flux}} \\ & + \underbrace{f_{DOPL}^{BME}(A, M, Z, F, 0)}_{\text{d-biological mort/excr}} \end{aligned} \quad (5.47)$$

$$\frac{\partial DOPR}{\partial t} = \underbrace{f_{POPR}^{DEC}(T, DO, POPR)}_{\text{a-POPR decomposition}} - \underbrace{f_{DOPR}^{MIN}(T, DO, B^*, DOPR)}_{\text{b-DOPR mineralization}} + \underbrace{f_{DOPR}^{DSF}(T, DO, pH)}_{\text{c-sediment flux}} \quad (5.48)$$

$$\begin{aligned} \frac{\partial POPL}{\partial t} = & - \underbrace{f_{POPL}^{DEC}(T, DO, B^*, POPL)}_{\text{a-POPL decomposition}} + \underbrace{f_{POPL}^{SET}(POPL)}_{\text{b-settling}} + \underbrace{f_{POPL}^{RES}(POPL_{sed})}_{\text{c-resuspension}} \\ & + \underbrace{f_{POPL}^{BME}(A, M, Z, F, 0)}_{\text{d-biological mort/excr}} - \underbrace{f_{POPL}^{GRZP}(Z, F, POPL)}_{\text{e-grazing}} + \underbrace{\sum_z k_{mfz} G_P(Z_z)}_{\text{f-zoop messy feeding}} + \underbrace{\sum_f k_{mff} G_P(F_f)}_{\text{g-fish messy feeding}} \end{aligned} \quad (5.49)$$

$$\frac{\partial POPR}{\partial t} = - \underbrace{f_{POPR}^{DEC}(T, DO, B^*, POPR)}_{\text{a-POPR decomposition}} + \underbrace{f_{POPR}^{SET}(POPR)}_{\text{b-settling}} + \underbrace{f_{POPR}^{RES}(POPR_{sed})}_{\text{c-resuspension}} \quad (5.50)$$

$$\frac{\partial PIP}{\partial t} = - \underbrace{f_{PO4,PIP}^{ADD}(SS1, SS2, PO_4, PIP)}_{\text{a-adsorption/desorption}} + \underbrace{f_{PIP}^{SET}(PIP)}_{\text{b-settling}} + \underbrace{f_{PIP}^{RES}(PIP_{sed})}_{\text{c-resuspension}} \quad (5.51)$$

$$\frac{\partial BIP}{\partial t} = \underbrace{U_{DOPL}(B)}_{\text{a-uptake}} + \underbrace{U_{FRP}(B)}_{\text{b-excretion}} - \underbrace{E_{FRP}(B)}_{\text{c-settling}} + \underbrace{f_B^{SET}(B)}_{\text{d-resuspension}} + \underbrace{f_B^{RES}(BIP_{sed})}_{\text{e-grazing}} - \underbrace{f_B^{GRZP}(Z, F, B)}_{\text{e-grazing}} \quad (5.52)$$

$$\begin{aligned} \frac{\partial AIP_a}{\partial t} = & \underbrace{U_{PO4}(A_a)}_{\text{a-uptake}} - \underbrace{E_{DOPL}(A_a) - E_{POPL}(A_a)}_{\text{b-mortality \& excretion}} + \underbrace{f_{A_a}^{SET}(AIP_a)}_{\text{c-settling}} + \underbrace{f_{A_a}^{RES}(AIP_{sed})}_{\text{d-resuspension}} \\ & - \underbrace{f_{A_a}^{GRZP}(Z, F, A_a)}_{\text{e-grazing}} \end{aligned} \quad (5.53)$$

$$\frac{\partial ZIP_z}{\partial t} = \underbrace{(1 - k_{mfz}) G_P(Z_z)}_{\text{a-grazing}} - \underbrace{E_{DOPL}(Z_z) - E_{POPL}(Z_z)}_{\text{b-excretion \& mortality}} - \underbrace{f_{Z_z}^{GRZP}(Z, F, Z_z)}_{\text{c-predation}} \quad (5.54)$$

$$\frac{\partial FIP_f}{\partial t} = \underbrace{(1 - k_{mff}) G_P(F_f)}_{\text{a-grazing}} - \underbrace{E_{DOPL}(F_f) - E_{POPL}(F_f)}_{\text{b-excretion \& mortality}} - \underbrace{f_{F_f}^{GRZP}(0, F, F_f)}_{\text{c-predation}} \quad (5.55)$$

$$TP = FRP + DOPL + DOPR + POPL + POPR + BIP + \sum_a^{N_A} AIP_a + \sum_z^{N_Z} ZIP_z \quad (5.56)$$

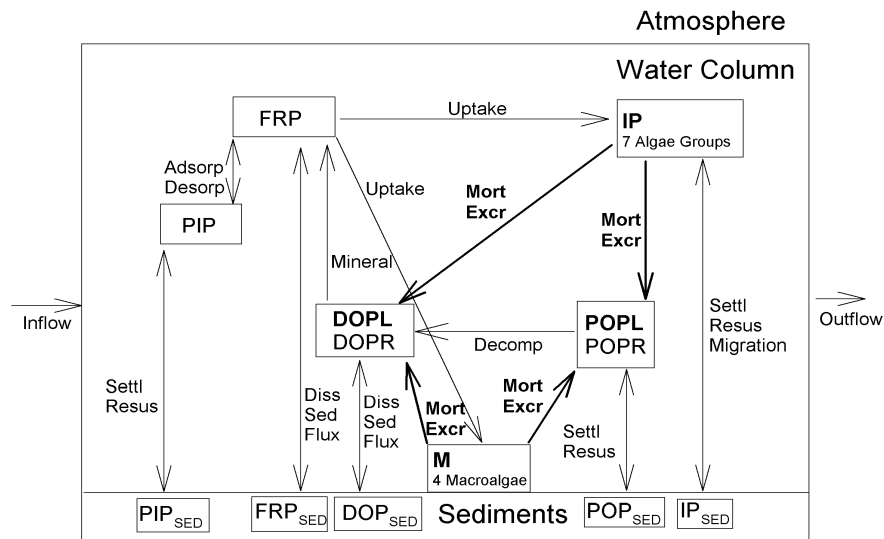


Figure 5.3 Simplified schematic of the phosphorus dynamics with CAEDYM.

6. Biological mortality and excretion into the *DOPL* and *POPL* pools.
7. Settling of *POPL*, *POPR*, *PIP* and *AIP*.
8. Resuspension of *POPL*, *POPR*, *PIP* and *AIP*.
9. Grazing of *POPL*, *POPR*, *BIP* and *AIP* by fish and zooplankton.

5.5 Nitrogen

At least five (if only one algal group and up to 11 with 7 algal groups) mandatory and numerous optional (refractory organics, particulate inorganic, and higher biology) nitrogen state variables are tracked by CAEDYM (Table 5.6). A schematic process representation (Figure 5.4) illustrates that the sources of the labile forms include fresh senescent organic material, whereas the refractory do not. The governing partial differential equations of all the processes of nitrogen transformations in the sediments and water column are summarized in Table 5.7.

The main processes involved in nitrogen fate in the sediments and water column are:

1. Mineralization of *DONL* and *DONR* to NH_4 .
2. Biological uptake of NH_4 and NO_3 by phytoplankton and macroalgae into the *IN* pool.
3. Dissolved sediment fluxes of NH_4 , NO_3 , *DONL*, and *DONR*.
4. Adsorption/desorption of NH_4 onto inorganic suspended solids into *PIN* pool.
5. Decomposition of *PONL* to *DONL* and *PONR* to *DONR*.
6. Biological mortality and excretion into the *DONL* and *PONL* pools.
7. Settling of *PONL*, *PONR*, *PIN* and *IN*.

Table 5.6 Nitrogen state variables simulated by CAEDYM. Modelled mechanisms for each state variable are provided. Macroalgae and all other biotic state variables have internal stores of N tracked. Sediment state variables mass balance is maintained with interactions with the water column, however no sediment transformations occur.

Variable	Name	Process Description
Mandatory State Variables:		
NO3	Nitrate + Nitrite	Equation 5.58: <i>Autotrophic uptake, mineralization, sediment flux, nitrification/denitrification</i>
NH4	Ammonium	Equation 5.57: <i>Autotrophic uptake, mineralization, nitrification, sediment flux, adsorption/desorption</i>
DONL	Labile Dissolved Organic Nitrogen	Equation 5.59: <i>Mineralization, decomposition of POPL, algal mortality/excretion, sediment flux, zooplankton & fish contribution</i>
PONL	Labile Particulate Organic Nitrogen	Equation 5.61: <i>Decomposition to DOPL, settling, algal mortality/excretion, resuspension, zooplankton & fish fluxes</i>
IN	Algal Internal Nitrogen (1 compulsory group, upto 7 available)	Equation ??: <i>Algal uptake, N₂ fixation, settling, resuspension, algal excretion/mortality, zooplankton & fish grazing</i>
Optional State Variables:		
DONR	Refractory Dissolved Organic Nitrogen	Equation 5.60: <i>Mineralization, decomposition of PONR, sediment flux</i>
PONR	Refractory Particulate Organic Nitrogen	Equation 5.62: <i>Decomposition to DONR, settling, resuspension</i>
PIN	Particulate Inorganic Nitrogen	Equation 5.63: <i>Adsorption/desorption, settling, resuspension</i>
BIN	Bacterial Internal Nitrogen	Equation 5.52: <i>Uptake, excretion, settling, resuspension, grazing</i>
ZIN	Zooplankton Internal Nitrogen (0 compulsory groups, upto 5 available)	Equation 5.54: <i>Grazing, excretion, mortality, predation</i>
FIN	Fish Internal Nitrogen (0 compulsory groups, upto 3 available)	Equation 5.55: <i>Grazing, excretion, mortality, predation</i>

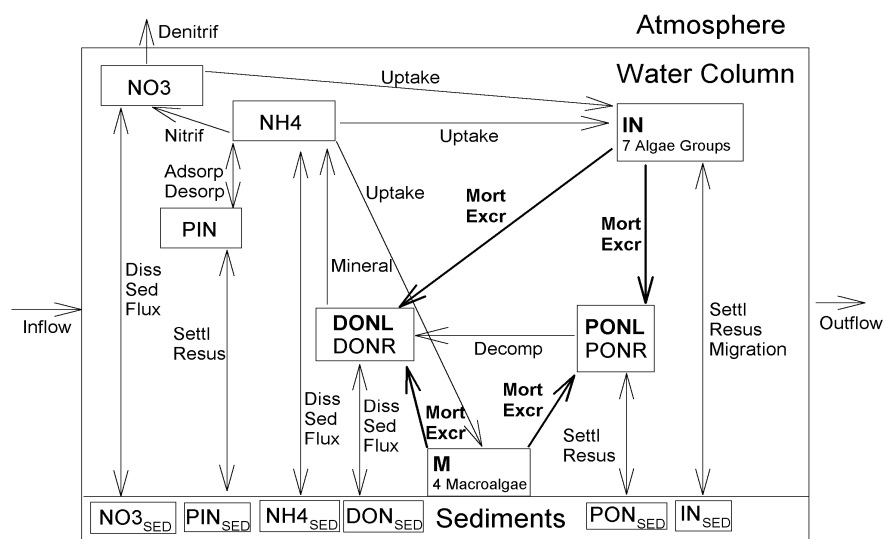


Figure 5.4 Simplified schematic of the nitrogen dynamics with CAEDYM.

Table 5.7 CAEDYM nitrogen cycle. All state variables also have source of inflows and loss via outflows and are subject to advection and mixing by the hydrodynamic driver.

$$\begin{aligned}
\frac{\partial NH_4}{\partial t} &= \underbrace{f_{DONL}^{MIN}(T, DO, DONL)}_{\text{a-labile DON minrzn (if bacf=F)}} + \underbrace{f_{DONR}^{MIN}(T, DO, DONR)}_{\text{b-refrac DON minrzn (if bacf=F)}} + \underbrace{f_{NH_4}^{BME}(0, 0, 0, 0, B)}_{\text{c-bacterial minrzn (if bacf=T)}} \\
&+ \underbrace{f_{NH_4}^{DSF}(T, DO, pH)}_{\text{d-sediment flux}} + \underbrace{f_{NH_4, PIN}^{ADD}(SS1, SS2, NH_4, PIN)}_{\text{e-adsorption/desorption}} - \underbrace{f_{NH_4}^{BUP}(A, M, B, NH_4)}_{\text{f-biological uptake}} \\
&- \underbrace{\mu_{NIT} f_{NIT}^{T_2}(T) f_{NIT}^{DO_1}(DO) NH_4}_{\text{g-nitrification}} \tag{5.57}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial NO_3}{\partial t} &= \underbrace{f_{NO_3}^{BUP}(A, M, B, NO_3)}_{\text{a-biological uptake}} + \underbrace{f_{NO_3}^{DSF}(T, DO, pH)}_{\text{b-sediment flux}} \\
&+ \underbrace{\mu_{NIT} f_{NIT}^{T_2}(T) f_{NIT}^{DO_1}(DO) NH_4}_{\text{c-nitrification}} - \underbrace{\mu_{DEN} f_{DEN}^{T_2}(T) f_{DEN}^{DO_2}(DO) NO_3}_{\text{d-denitrification}} \tag{5.58}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial DONL}{\partial t} &= \underbrace{f_{PONL}^{DEC}(T, DO, B^*, PONL)}_{\text{a-PONL decomposition}} - \underbrace{f_{DONL}^{MIN}(T, DO, DONL)}_{\text{b-DONL mineralization}} \\
&+ \underbrace{f_{DONL}^{DSF}(T, DO, pH)}_{\text{c-sediment flux}} + \underbrace{f_{DONL}^{BME}(A, M, Z, F)}_{\text{d-biological mort/excr}} - \underbrace{f_{DONL}^{BUP}(0, 0, B, DONL)}_{\text{e-bacterial uptake}} \tag{5.59}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial DONR}{\partial t} &= \underbrace{f_{PONR}^{DEC}(T, DO, B^*, PONR)}_{\text{a-PONR decomposition}} - \underbrace{f_{DONR}^{MIN}(T, DO, DONR)}_{\text{b-DONR mineralization}} - \underbrace{f_{DONR}^{DSF}(T, DO, pH)}_{\text{c-sediment flux}} \tag{5.60}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial PONL}{\partial t} &= - \underbrace{f_{PONL}^{DEC}(T, DO, B^*, PONL)}_{\text{a-PONL decomposition}} + \underbrace{f_{PONL}^{SET}(PONL)}_{\text{b-settling}} + \underbrace{f_{PONL}^{RES}(PONL_{sed})}_{\text{c-resuspension}} \\
&+ \underbrace{f_{PONL}^{BME}(A, M, Z, F, 0)}_{\text{d-biological mort/excr}} - \underbrace{f_{POPL}^{GRZN}(Z, F, PONL)}_{\text{e-grazing}} + \underbrace{\sum_z k_{mfz} G_N(Z_z)}_{\text{f-zoop messy feeding}} + \underbrace{\sum_f k_{mff} G_N(F_f)}_{\text{g-fish messy feeding}} \tag{5.61}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial PONR}{\partial t} &= - \underbrace{f_{PONR}^{DEC}(T, DO, B^*, PONR)}_{\text{a-PONR decomposition}} + \underbrace{f_{PONR}^{SET}(PONR)}_{\text{b-settling}} + \underbrace{f_{PONR}^{RES}(PONR_{sed})}_{\text{c-resuspension}} \tag{5.62}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial PIN}{\partial t} &= - \underbrace{f_{NH_4, PIN}^{ADD}(SS1, SS2, NH_4, PIN)}_{\text{a-adsorption/desorption}} + \underbrace{f_{PIN}^{SET}(PIN)}_{\text{b-settling}} + \underbrace{f_{PIN}^{RES}(PIN_{sed})}_{\text{c-resuspension}} \tag{5.63}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial BIN}{\partial t} &= \underbrace{U_{DONL}(B) + U_{NO_3}(B) + U_{NH_4}(B)}_{\text{a-uptake}} - \underbrace{E_{NH_4}(B)}_{\text{b-excretion}} + \underbrace{f_B^{SET}(B)}_{\text{c-settling}} + \underbrace{f_B^{RES}(BIN_{sed})}_{\text{d-resuspension}} \\
&- \underbrace{f_B^{GRZN}(Z, F, B)}_{\text{e-grazing}} \tag{5.64}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial AIN_a}{\partial t} &= \underbrace{U_{NH_4}(A_a) + U_{NO_3}(A_a)}_{\text{a-uptake}} + \underbrace{f_{A_a}^{NFx}(A_a, NO_3, NH_4)}_{\text{b-N}_2 \text{ fixation}} - \underbrace{E_{DONL}(A_a) - E_{PONL}(A_a)}_{\text{c-mortality \& excretion}} \\
&+ \underbrace{f_{A_a}^{SET}(AIN_a)}_{\text{d-settling}} + \underbrace{f_{A_a}^{RES}(AIN_{sed})}_{\text{e-resuspension}} - \underbrace{f_{A_a}^{GRZN}(Z, F, A_a)}_{\text{f-grazing}} \tag{5.65}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial ZIN_z}{\partial t} &= \underbrace{(1 - k_{mfz}) G_N(Z_z)}_{\text{a-grazing}} - \underbrace{E_{DONL}(Z_z) - E_{PONL}(Z_z)}_{\text{b-excretion \& mortality}} - \underbrace{f_{Z_z}^{GRZN}(Z, F, Z_z)}_{\text{c-predation}} \tag{5.66}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial FIN_f}{\partial t} &= \underbrace{(1 - k_{mff}) G_N(F_f)}_{\text{a-grazing}} - \underbrace{E_{DONL}(F_f) - E_{PONL}(F_f)}_{\text{b-excretion \& mortality}} - \underbrace{f_{F_f}^{GRZN}(0, F, F_f)}_{\text{c-predation}} \tag{5.67}
\end{aligned}$$

$$TN = NH_4 + NO_3 + DONL + DONR + PONL + PONR + BIN + \sum_a^{N_A} AIN_a + \sum_z^{N_Z} ZIN_z \tag{5.68}$$

Table 5.8 Silica state variables simulated by CAEDYM. Modelled mechanisms for each state variable are provided.

Variable	Name	Process Description
Optional State Variables:		
SiO2	Dissolved Silica	Equation 5.69: <i>Diatom uptake and loss, sediment flux</i>
ISi	Algal Internal Silica	Equation 5.70: <i>Diatom uptake/mortality/excretion, settling, resuspension</i>

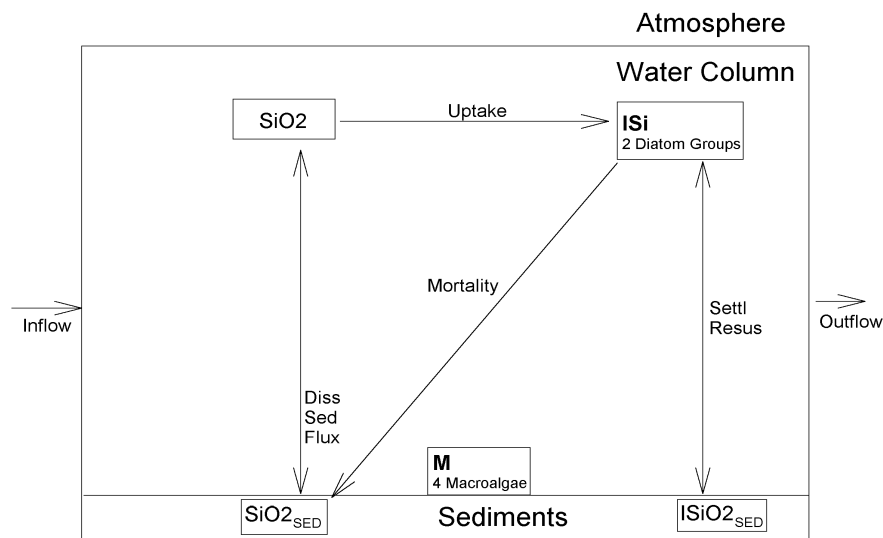


Figure 5.5 Simplified schematic of the carbon dynamics with CAEDYM.

8. Resuspension of *PONL*, *PONR*, *PIN* and *IN*.
9. Nitrification of NH_4 to NO_3 .
10. Denitrification of NO_3 to N_2 (note that N_2 is not tracked by CAEDYM).
11. N_2 fixation (note that N_2 is not tracked by CAEDYM).
12. Grazing of *PONL*, *PONR*, *BIN* and *AIN* by zooplankton and fish.

5.6 Silica

Up to 3 (if 2 diatom groups simulated) silica state variables are tracked by CAEDYM (Table 5.8). The necessary silica state variables are automatically simulated within CAEDYM if either or both of the diatom species are selected (phytoplankton groups 6 and 7), otherwise silica is not modelled. A schematic process representation (Figure 5.5) illustrates that the sources of the labile forms include fresh senescent organic material, whereas the refractory do not have these sources. The governing partial differential equations of all the processes of carbon fate in the sediments and water column are summarized in Table 5.9.

The main processes involved in silica fate in the sediments and water column are:

Table 5.9 CAEDYM silica cycle. All state variables also have source of inflows and loss via outflows and are subject to advection and mixing by the hydrodynamic driver.

$$\frac{\partial SiO_2}{\partial t} = - \underbrace{f_{SiO_2}^{BUP}(A, 0, 0, SiO_2)}_{\text{a-diatom uptake}} + \underbrace{f_{SiO_2}^{DSF}(T, DO, pH)}_{\text{b-sediment flux}} \quad (5.69)$$

$$\frac{\partial ISi}{\partial t} = \underbrace{f_{SiO_2}^{BUP}(A, 0, 0, SiO_2)}_{\text{a-diatom uptake}} - \underbrace{f_{SiO_2}^{BME}(A, 0, 0, 0, 0)}_{\text{b-diatom mort/excr}} + \underbrace{f_{ISi}^{SET}(ISi)}_{\text{c-settling}} + \underbrace{f_{ISi}^{RES}(ISi_{sed})}_{\text{d-resuspension}} \quad (5.70)$$

1. Biological uptake of SiO₂ by diatoms into the ISi pool.
2. Dissolved sediment fluxes of SiO₂.
3. Biological mortality directly in the SiO₂ sediment pool. The assumption is that the diatom frustules rapidly settle into the sediments and are rapidly mineralized in the sediments.
4. Settling of ISi.
5. Resuspension of ISi.

5.7 Bacteria

Bacterial biomass can optionally be modelled within CAEDYM (set: bacf = T), through the state variable B (Eq. 5.22). If bacteria are not explicitly simulated, they are still assumed to mediate the mineralization of organic matter, but CAEDYM will directly flux DOM to the DIM pool and the conversion rate will not dynamically account for the affect of bacterial abundance or limitation. For most applications it is generally unnecessary to include this functionality.

As with the other biological state variables, carbon is considered the key currency of bacterial biomass, but the internal concentrations of bacterial N and P are also modelled using a fixed stoichiometric ratio (Si is currently not included). The uptake and loss functions required for the bacteria mass balance equations are outlined next.

The bacteria model operates by assuming they first consume any dissolved organic matter; for carbon this is modelled as:

$$U_{DOC}(B) = f_{DOC}^{DEC}(T, DO, B, DOC) \quad (5.71)$$

where the decomposition function is outline in Table 5.1. Nitrogen and phosphorus are taken up to match this, but if insufficient DON or DOP exists, then they can also take up the inorganic form. This is written as:

$$U_{DOP}(B) = \begin{cases} U_{DOC}(B) k_{BIP} & DOP > U_{DOC}(B) k_{BIP} \\ DOP & DOP \leq U_{DOC}(B) k_{BIP} \end{cases} \quad (5.72)$$

$$U_{DON}(B) = \begin{cases} U_{DOC}(B) k_{BIN} & DON > U_{DOC}(B) k_{BIN} \\ DON & DON \leq U_{DOC}(B) k_{BIN} \end{cases} \quad (5.73)$$

$$U_{FRP}(B) = \begin{cases} U_{DOC}(B) k_{BIP} - U_{DOP}(B) & U_{DOP}(B) < U_{DOC}(B) k_{BIP} \\ 0 & U_{DOP}(B) = U_{DOC}(B) k_{BIP} \end{cases} \quad (5.74)$$

$$U_{NH_4}(B) = \begin{cases} NH_4 & U_{DOC}(B) k_{BIN} > (DON + NH_4) \\ U_{DOC}(B) k_{BIN} - U_{DON}(B) & U_{DON}(B) \leq U_{DOC}(B) k_{BIN} \\ 0 & U_{DON}(B) = U_{DOC}(B) k_{BIN} \end{cases} \quad (5.75)$$

$$U_{NO_3}(B) = \begin{cases} NO_3 & U_{DOC}(B) k_{BIN} > (DON + NH_4 + NO_3) \\ U_{DOC}(B) k_{BIN} - U_{DON}(B) - U_{NH_4}(B) & U_{DON}(B) + U_{NH_4}(B) \leq U_{DOC}(B) k_{BIN} \\ 0 & U_{DON}(B) + U_{NH_4}(B) = U_{DOC}(B) k_{BIN} \end{cases} \quad (5.76)$$

Note also, that If bacteria are configured, then the microbial decomposition process of particulate organic matter also have the bacterial biomass dependence added into the rate calculation (Eq. 5.9).

Loss process for the bacteria are modelled as:

$$R_{DIC}(B) = k_{r_B} f_B^{T^2}(T) B \quad (5.77)$$

for respiration, where $k_{r_{BAC}}$ is the respiration rate of bacteria (day^{-1}), and for excretion (or mineralization):

$$E_{DOCL}(B) = k_{B_e} U_{DOC}(B) \quad (5.78)$$

$$E_{FRP}(B) = [R_{DIC}(B) + E_{DOCL}(B)] k_{BIP} \quad (5.79)$$

$$E_{NH_4}(B) = [R_{DIC}(B) + E_{DOCL}(B)] k_{BIN}. \quad (5.80)$$

Biological Variables (Water Column)

6.1 Introduction

CAEDYM allows for the configuration of several groups of ‘water column’ biology:

1. 1-7 phytoplankton groups (Section 6.2);
2. 0-5 zooplankton groups (Section 6.3);
3. 0-3 fish groups (Section 6.4);
4. 0-1 jellyfish groups (Section 6.5);

The term ‘water column’ biology is used to differentiate these species from the benthic biological species discussed in Chapter 7; the essential difference between the two is that the water column species are modelled in each wet cell, whereas the benthic species are only modelled in the bottom layer (i.e. cells adjacent to the sediment). The elemental balance equations for each of these groups of variables are presented in Chapter 5. Each of processes outlined in these tables are discussed throughout the chapter, and the necessary parameterizations are discussed.

6.2 Phytoplankton

There are seven phytoplankton groups configurable within CAEDYM. Although the seven groups are **generic** and operate within the model **identically** (with the exception of groups 6 & 7, which also include internal silica stores and silica growth dependence), as a guide the 7 state variables are intended to represent the groups as described in Table 6.1, but may be configured any way the user would like.

Phytoplankton biomass is represented in terms of chlorophyll-a ($\mu\text{g Chla } L^{-1}$) or in terms of carbon ($\text{mg } C L^{-1}$) depending on the user configuration (set: CorChla). Note however, that throughout this chapter chlorophyll-a units are assumed - where ‘carbon currency’ is used, the conversion from chlorophyll to carbon should be ignored. In the elemental cycle descriptions (Chapter 5), phytoplankton biomass is considered to be in carbon currency despite which units the user selects.

Algal involvement in the nutrient cycles is depicted schematically in the previous chapter. Figure 6.1 provides an overview of algal dynamics as modelled by CAEDYM. The balance equations for algal nutrients are also presented in the previous chapter, and the various parameterisations used in those equations are described next. Note that at present there is no representation of heterotrophy in any of the phytoplankton groups. Such a representation would require a change to the source code of the CAEDYM model.

6.2.1 Growth: For each phytoplankton group, the maximum potential growth rate at $20^{\circ}C$ is multiplied by the minimum value of expressions for limitation by light, phosphorus, nitrogen and, when diatoms are considered,

Table 6.1 Description of the seven phytoplankton groups configurable within CAEDYM.

Group, <i>a</i>	Identifier	Description
1	DINOF	Dinoflagellates: may be either freshwater (e.g. <i>Peridinium</i> sp.) or estuarine/marine species (e.g. <i>Gymnodinium</i> sp.). Motility is a prominent feature of this group and is included in CAEDYM as a process representation.
2	CYANO	Freshwater cyanobacteria: The main process represented in this group is buoyancy control. As a broad generalisation this group is suited to quiescent, warm, stratified conditions. Nitrogen fixation (e.g. by <i>Anabaena</i>) can be simulated explicitly. A typical genus constituting this group is <i>Microcystis</i> sp.
3	NODUL	Marine/estuarine cyanobacteria: This group is represented by <i>Nodularia</i> sp., which has a wide salinity tolerance. The process representation for this group includes buoyancy regulation. In some applications of the model to freshwaters, the user may wish to simulate a second freshwater cyanobacterial group. This is possible by specifying a freshwater case and also denoting this group as a state variable. For example, the user might wish to examine succession of the freshwater cyanobacteria <i>Anabaena circinalis</i> and <i>Microcystis aeruginosa</i> in a lake, and would therefore require the two cyanobacterial groups to be simulated.
4	CHLOR	Chlorophytes: A typical member of this group is the freshwater alga <i>Chlamydomonas</i> sp. This group is typically freshwater, but there is provision in the model for the group to be estuarine or marine as required. Motility in this group is included as a process representation in the CAEDYM model.
5	CRYPT	Cryptophytes: This group can be included either as freshwater, estuarine or marine by the appropriate specification. Motility in this group is included as a process representation in CAEDYM. The model gives flexibility to simulate up to seven groups and can be switched between fresh, estuarine or marine waters by allocating the salinity of the waterbody as a general input or by adjusting the salinity dependence of the different phytoplankton species state variables individually.
6	MDIAT	Marine/estuarine diatoms: Process representations and assumptions included in CAEDYM are identical to those for freshwater diatoms, but with different salinity response. Example: <i>Skeletonema</i> sp.
7	FDIAT	Freshwater diatoms: Process representations included in CAEDYM are: silica dependence and intolerance to salinity. This group is considered to be non-motile, e.g. <i>Synedra</i> .

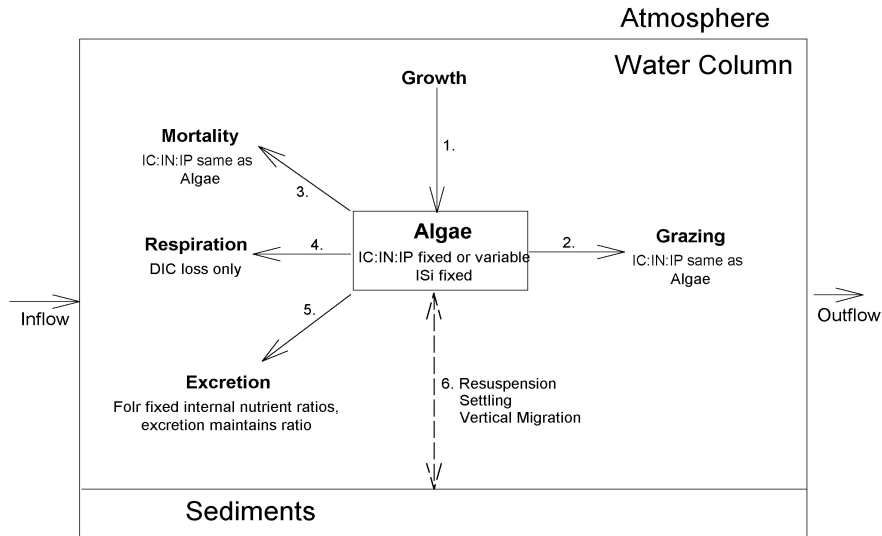


Figure 6.1 Schematic of phytoplankton dynamics within CAEDYM.

silica. While there may be some interaction between limiting factors, a minimum expression is likely to provide a realistic representation of growth limitation (Rhee and Gotham, 1981), especially over the relatively small spatial and temporal scales that are to be used for most phytoplankton simulations.

The growth rate, μ_g (day^{-1}) is therefore modelled as:

$$\mu_{g_a} = \mu_{MAX_a} \min [f(I)_a, f(N)_a, f(P)_a, f(Si)_a^*, f(C)_a^{**}] f_{A_a}^{T1}(T) \quad (6.1)$$

where $f(I)$, $f(N)$ and $f(P)$ represent limitation by light, nitrogen and phosphorus respectively, f^{T1} is a temperature function defined previously and μ_{max} (day^{-1}) is the maximum growth rate at $20^\circ C$ in the absence of significant limitation by light or nutrients. Note that μ_{MAX} includes photorespiration effects inherently and a separate term for this effect is not warranted. Each of the functions are described in more detail below.

*: $f(Si)$ represents limitation by silica and applies only to diatoms ($a = 6, 7$).

** : $f(C)$ is used where the internal carbon store is modelled explicitly (see the carbon section below). In such a case the $f(C)$ term will replace the $f(I)$ term - the relation between $f(I)$ and $f(C)$ is given below.

Light: There are two different models for quantifying the effects of light limitation of phytoplankton. The term light is used loosely here to refer to photosynthetically active radiation (PAR) in the waveband $400-700nm$. The majority of applications are likely to involve data collected for total daily shortwave radiation. These data are converted to photosynthetically active radiation (PAR), based on 45% of net incoming shortwave radiation being in the photosynthetically active wavelength (Jellison and Melack, 1993). A brief description of methods of input of shortwave radiation is discussed in section 2.

In the absence of significant photoinhibition (set: algt=2), the model of Webb et al. (1974) can be used to quantify the fractional limitation of the growth rate by light:

$$f(I) = 1 - \exp\left(\frac{-I}{I_k}\right) \quad (6.2)$$

where the term $f(I)$ equates to μ_g/μ_{MAX} , where μ_g is the rate of carbon fixation and μ_{MAX} is the maximum potential rate of carbon fixation, I is the incoming irradiance and I_k is the light intensity at which the photosynthetic rate is numerically equivalent to μ_{MAX} if light saturation behavior was absent (Talling, 1957). The equations are then integrated with respect to the depth, z , which refers to the grid cell depth for ELCOM, or the layer thickness for DYRESM. The depth integral of the Webb model is calculated as follows:

$$\begin{aligned} \text{Let } P^* &= \mu/\mu_{MAX} = f(I) \\ I^* &= I_o/I_k \\ z^* &= \eta z, \end{aligned}$$

so the Webb model can be written as:

$$P^* = 1 - \exp[-I^* \exp(-Z^*)]. \quad (6.3)$$

Now consider the depth integrated form:

$$\begin{aligned} \text{Let } g &= \int_{z_1}^{z_2} P(z) dz \\ z &= z^*/\eta \\ dz &= dz^*/\eta, \end{aligned}$$

leaving:

$$\eta g = \int_{z_1}^{z_2} P(z^*) dz^*. \quad (6.4)$$

If we now define $\eta g/P_{max} = g^*$, and substitute:

$$\begin{aligned} g^* &= \int_{z_1}^{z_2} [1 - \exp(-I^* \exp(-z^*))] dz^* \\ &= [z^* + E_i(-I^* \exp(-z^*))]_{z_1^*}^{z_2^*} \end{aligned} \quad (6.5)$$

where:

$$E_i(\beta) = \int_{-x}^{\beta} \frac{e^{\bar{\beta}}}{\bar{\beta}} d\bar{\beta}, \quad (6.6)$$

and calculation of $E_i(\beta)$ is done using a numerical approximation method, as described in Spanier and Oldham (1987).

For the case of light saturation (set: algt=3), the model takes the form:

$$f(I) = \frac{I}{I_s} \exp\left(1 - \frac{I}{I_s}\right) \quad (6.7)$$

where I_s represents the light saturation value at which production is maximal. A depth integral is again used for the above equation, following the method of Wallace et al. (1996). In the above two cases the value of $f(I)$ is not integrated over time, but I is integrated over time. Over time steps of 3 hours or less, the difference between the integrated I and the integrated $f(I)$ term is insignificant in terms of the value of $f(I)$.

Temperature: To allow for inhibition of phytoplankton at higher temperatures, a temperature function is used where maximum productivity occurs at a temperature T_{OPT} , above which productivity decreases to zero at temperature T_{MAX} . Below the temperature T_{STD} the productivity follows the normal relation, f^{T2} :

$$f_{A_a}^{T2}(T) = \vartheta_{A_a}^{T-20} \quad (6.8)$$

These restrictions require the following conditions be imposed:

- (1). at $T = T_{STD}$: $f(T) = 1$;
- (2). at $T = T_{OPT}$: $\frac{\partial f(T)}{\partial t} = 0$;
- (3). at $T = T_{MAX}$: $f(T) = 0$.

CAEDYM assumes a function of the form:

$$f^{T1}(T) = \vartheta^{T-20} - \vartheta^{k(T-a)} + b \quad (6.9)$$

where k , a and b are unknown, then from the first condition:

$$b = 2 + \vartheta^{k(T_{STD}-a)} - \vartheta^{T_{STD}-20}, \quad (6.10)$$

and from conditions 2 and 3:

$$\begin{aligned} a &= -\ln \left[\frac{\vartheta^{T_{STD}-20} - \vartheta^{T_{MAX}-20}}{\vartheta^{kT_{STD}} - \vartheta^{kT_{MAX}}} \right] \frac{1}{k \ln(\vartheta)} \\ &= -\ln \left[\frac{\vartheta^{T_{OPT}-20}}{\vartheta^{kT_{OPT}}} \right] \frac{1}{k \ln(\vartheta)}. \end{aligned} \quad (6.11)$$

$$(6.12)$$

This results in an equation for the unknown, k , as given by:

$$G(k) = k\vartheta^{kT_{OPT}} (\vartheta^{T_{STD}-20} - \vartheta^{T_{MAX}-20} - 1) - \vartheta^{T_{OPT}-20} (\vartheta^{kT_{STD}} - \vartheta^{kT_{MAX}}), \quad (6.13)$$

which is solved numerically for k via Newton's method, where the initial approximation to the root is $k = 6.0$. The unknowns a and b are calculated later. Using typical values of $T_{STD} = 20$, $T_{OPT} = 33$ and $T_{MAX} = 39^\circ C$, then $k = 4.02$, $a = 34.26$ and $b = 0.012$. The function $f^{T1}(T)$ closely follows the curve ϑ^{T-20} for $T < T_{STD}$, attains a maximum of 2.1 at T_{OPT} and decreases smoothly to reach zero at T_{MAX} . For some choices of T_{OPT} and T_{MAX} , $f^{T1}(T)$ may deviate slightly from the curve ϑ^{T-20} for $T < T_{STD}$, but this deviation is minimal.

Nitrogen: There are two options available to the user to model nitrogen dynamics within the algal groups:

1. Constant, user-defined nitrogen concentration, or
2. Dynamic intracellular store which is able to regulate growth.

For the first model, a simple Michaelis-Menten equation is used to model nitrogen limitation:

$$f(N)_a = \frac{NH_4 + NO_3}{NH_4 + NO_3 + K_{N_a}} \quad (6.14)$$

where K_N is the half-saturation constant for the effect of nitrogen on the growth rate. Nitrogen uptake during growth is then simply the growth rate multiplied by the user-defined internal nitrogen ratio, k_{AIN} :

$$U_{NH_4}(A_a) = P_{N_a} k_{AIN_a} \mu_g \quad (6.15)$$

$$U_{NO_3}(A_a) = (1 - P_{N_a}) k_{AIN_a} \mu_g \quad (6.16)$$

where P_{N_a} is the preference of the a^{th} group for NH_4 (between 0 and 1) and is defined according to the relative abundance of the inorganic nitrogen species:

$$P_N = \frac{NH_4 NO_3}{(NH_4 + K_N)(NO_3 + K_N)} + \frac{NH_4 K_N}{(NH_4 + NO_3)(NO_3 + K_N)}. \quad (6.17)$$

For this simple model, metabolic loss of nitrogen (via mortality and excretion) is the constant internal nitrogen ratio multiplied by the loss rate:

$$E_{DONL}(A_a) = f_{DOM} [k_{AIN_a} L_a f(S)_a] \quad (6.18)$$

$$E_{PONL}(A_a) = (1 - f_{DOM}) [k_{AIN_a} L_a f(S)_a] \quad (6.19)$$

where f_{DOM} is the fraction of excretion and mortality that enters the dissolved organic matter (DOM) pool, and the loss rate, L , is discussed in more detail below. Although for this model no internal nitrogen state variable is actually instantiated within CAEDYM, the state equation described by 5.65 still applies but is modelled implicitly (i.e no state variable is generated and transported).

The dynamic internal nutrient model is more parameter expensive, but does allow for the phytoplankton to have variable internal nitrogen concentrations. Under this model, the limitation function takes the form:

$$f(N)_a = \frac{AIN_{MAX_a}}{AIN_{MAX_a} - AIN_{MIN_a}} \left[1 - \frac{AIN_{MIN_a}}{AIN_a} \right] \quad (6.20)$$

where AIN_{MAX} and AIN_{MIN} are user-defined bounds for the internal nitrogen concentrations. Using this method the internal nitrogen store for each phytoplankton group is specified as a unique state variable within CAEDYM and is advected and settles with the phytoplankton and is grazed by zooplankton etc.. The internal store mass balance is modelled according to 5.65, and the uptake functions are modelled dynamically:

$$U_{NH_4}(A_a) = U_{N_{MAX_a}} P_{N_a} \left[f_{A_a}^{T1}(T) \frac{AIN_{MAX_a} - AIN_a}{AIN_{MAX_a} - AIN_{MIN_a}} \frac{NO_3 + NH_4}{NO_3 + NH_4 + K_{N_a}} \right] A_a \quad (6.21)$$

$$U_{NO_3}(A_a) = U_{N_{MAX_a}} (1 - P_{N_a}) \left[f_{A_a}^{T1}(T) \frac{AIN_{MAX_a} - AIN_a}{AIN_{MAX_a} - AIN_{MIN_a}} \frac{NO_3 + NH_4}{NO_3 + NH_4 + K_{N_a}} \right] A_a \quad (6.22)$$

where P_N is defined as above (6.17), UN_{MAX} is the maximum rate of nitrogen uptake ($mg\ N\ (mg\ Chla)^{-1}\ day^{-1}$), and A_a is the biomass of a^{th} phytoplankton group in chlorophyll-a units. The temperature function includes limitation at high temperatures and is identical to that used for phytoplankton growth (6.9). Nitrogen loss through mortality and excretion for the internal nutrient model is similar to the simple model described above (6.19), except that the dynamically calculated internal nutrient concentration is used:

$$E_{DONL}(A_a) = \left[\frac{AIN_a}{A_a} L_a f(S)_a \right] f_{DOM_a} \quad (6.23)$$

$$E_{PONL}(A_a) = \left[\frac{AIN_a}{A_a} L_a f(S)_a \right] (1 - f_{DOM_a}). \quad (6.24)$$

Note that settling and resuspension applies equally to the internal nitrogen concentration as to the algal chlorophyll-a/carbon concentrations for each group.

CAEDYM v2.1 and above allows users to model N_2 fixation for any algal group, as defined by the uptake function $U_{N_2}(A_a)$. Nitrogen fixation is considered to be optimal when the value of the nitrogen limitation function, $f(N)$, is zero, and it is minimum when $f(N)$ is 1. Note that although the limitation function is still calculated, it is only used as an indicator of the amount of dissolved inorganic nitrogen available; no actual N limitation is applied however. The user must provide the maximum nitrogen fixation rate, $k_{NF_{max}}$ ($mg\ N\ fixed\ (mg\ Chla)^{-1}\ day^{-1}$), which is the value when no NO_3 or NH_4 is present and when the internal nitrogen stores are depleted. The amount of nitrogen fixed for the i -th group is therefore:

$$U_{N_2}(A_a) = k_{NF_{max}} (1 - f(N)_a) A_a \quad (6.25)$$

such that the amount of fixation is optimum when no dissolved inorganic nitrogen is present. Of course, the metabolic capacity of the cells is compromised as the rate of nitrogen fixation increases, and the growth rate must therefore be reduced accordingly. The growth equation for nitrogen fixing algae is therefore written as:

$$\mu_{g_a} = \mu_{MAX_a} \min [f(I)_a, f(P)_a, f(Si)_a^*, f(C)_a^{**}] f_{A_a}^{T1}(T) [f_{NF_a} + f(N)_a (1 - f_{NF_a})] \quad (6.26)$$

where f_{NF_a} is the fraction of the maximum growth rate that is experienced under maximum nitrogen fixation. The nitrogen fixation model works with both the static and dynamic internal nitrogen options. For the latter, then the uptake functions for NO_3 and NH_4 are calculated as described above, and the total nitrogen intake is the sum of that taken up and the fixation component. For the static model however, a nitrogen uptake amount is dependent only on the μ_g . In this case, the amount of fixed nitrogen is calculated according to Eq. 6.25, and any shortfall is taken from the dissolved inorganic pool to maintain k_{AIN_a} :

$$U_{NH_4}(A_a) = P_{N_a} [k_{AIN_a} \mu_g - U_{N_2}(A_a)] \quad (6.27)$$

$$U_{NO_3}(A_a) = (1 - P_{N_a}) [k_{AIN_a} \mu_g - U_{N_2}(A_a)] \quad (6.28)$$

Phosphorus: There are two options available to the user to model phosphorus dynamics within the algal groups:

1. Constant, user-defined phosphorus concentration, or
2. Dynamic intracellular store that is able to regulate growth.

For the first model, a simple Michaelis-Menten equation is used to model phosphorus limitation:

$$f(P)_a = \frac{FRP}{FRP + K_{P_a}} \quad (6.29)$$

where K_P is the half-saturation constant for the effect of phosphorus on the growth rate. Phosphorus uptake during growth is then simply the growth rate multiplied by the user-defined internal phosphorus ratio, k_{AIP} :

$$U_{FRP}(A_a) = k_{AIP_a} \mu_{g_a}. \quad (6.30)$$

For this simple model, metabolic loss of phosphorus (via mortality and excretion) is the constant internal phosphorus ratio multiplied by the loss rate:

$$E_{DOPL}(A_a) = [k_{AIP_a} L_a f(S)_a] f_{DOM_a} \quad (6.31)$$

$$E_{POPL}(A_a) = [k_{AIP_a} L_a f(S)_a] (1 - f_{DOM_a}) \quad (6.32)$$

where f_{DOM} is the fraction of excretion and mortality that enters the dissolved organic matter (DOM) pool, and the loss rate, L , is discussed in more detail below. Although for this model no internal phosphorus state variable is actually instantiated within CAEDYM, the state equation described by 5.53 still applies but is modelled implicitly.

As with nitrogen, the dynamic internal phosphorus model is more parameter expensive, but does allow for the phytoplankton to have variable internal phosphorus concentrations. Under this model, the limitation function takes the form:

$$f(P)_a = \frac{AIP_{MAX_a}}{AIP_{MAX_a} - AIP_{MIN_a}} \left[1 - \frac{AIP_{MIN_a}}{AIP_a} \right] \quad (6.33)$$

where AIP_{MAX} and AIP_{MIN} are user-defined bounds for the internal phosphorus concentrations. Using this method the internal phosphorus store for each phytoplankton group is specified as a unique state variable within CAEDYM and is advected and settles with the phytoplankton and is grazed by zooplankton etc.. The internal store is modelled according to 5.53, and the uptake function is modelled dynamically:

$$U_{FRP}(A_a) = UP_{MAX_a} \left[f_{A_a}^{T1}(T) \frac{AIP_{MAX_a} - AIP_a}{AIP_{MAX_a} - AIP_{MIN_a}} \frac{FRP}{FRP + K_{P_a}} \right] A_a \quad (6.34)$$

where UP_{MAX} is the maximum rate of phosphorus uptake ($mg P (mg Chla)^{-1} day^{-1}$), and A_a is the biomass of a^{th} phytoplankton group in chlorophyll-a units. The temperature function includes limitation at high temperatures and is identical to that used for phytoplankton growth (6.9). Phosphorus loss through mortality and excretion

for the internal nutrient model is similar to the simple model described above (6.32), except that the dynamically calculated internal nutrient concentration is used:

$$E_{DOPL}(A_a) = \left[\frac{AIP_a}{A_a} L_a f(S)_a \right] f_{DOM_a} \quad (6.35)$$

$$E_{POPL}(A_a) = \left[\frac{AIP_a}{A_a} L_a f(S)_a \right] (1 - f_{DOM_a}) \quad (6.36)$$

Note that settling and resuspension applies equally to the internal nitrogen concentration as to the algal chlorophyll-a/carbon concentrations for each group.

Carbon: There are several methods available within CAEDYM to model the carbon dynamics of phytoplankton cells:

1. model the algal cells in chlorophyll-a units and prescribe a constant carbon to chlorophyll ratio, $Y_{C:Chla}$, in the parameters file;
2. model the algal cells in units of carbon directly (configured via the CorChla flag in the configuration file) - this method operates similar to that above, except input and output units are in carbon currency instead of chlorophyll-a currency;
3. the third option is to use an equation to vary the ratio of carbon to chlorophyll-a with physiological factors;
4. the last option is to explicitly model the carbon content of the cells, so that the carbon effectively acts as an internal nutrient.

The first model is recommended for most users. This operates similar to the simple models described above for nitrogen and phosphorus:

$$U_{DIC}(A_a) = Y_{C:Chla_a} \mu_{g_a} (1 - k_p) \quad (6.37)$$

$$R_{DIC}(A_a) = Y_{C:Chla_a} [f_{RES_a} L_a f(S)_a + k_p \mu_{g_a}] \quad (6.38)$$

$$E_{DOCL}(A_a) = [Y_{C:Chla_a} (1 - f_{RES_a}) L_a f(S)_a] f_{DOM_a} \quad (6.39)$$

$$E_{POCL}(A_a) = [Y_{C:Chla_a} (1 - f_{RES_a}) L_a f(S)_a] (1 - f_{DOM_a}) \quad (6.40)$$

where $U_{DIC}(A_a)$ is the uptake of CO_2 through photosynthesis, k_p is the photorespiration fraction, $R_{DIC}(A_a)$ is the amount of carbon lost to CO_2 through respiration by algal group a , f_{RES} is the fraction of the total metabolic loss, L , that is actual respiration and $E_{DOCL}(A_a)$ and $E_{POCL}(A_a)$, is therefore the carbon that is lost from the algal pool through mortality and excretion to DOCL and POCL respectively (refer to Table 5.3 for a complete overview of the carbon cycle). For the second model listed above, the above functions also apply, but without the carbon to chlorophyll-a conversion, $Y_{C:Chla}$.

The third model still simulates the phytoplankton in units of chlorophyll-a, however the ratio of carbon to chlorophyll is dynamic and calculated within CAEDYM depending upon the prevailing conditions. Therefore, equations 6.37-6.40 still apply, but rather than use a constant value of $Y_{C:Chla}$, it is calculated dynamically according to (Ambrose et al., 1988):

$$Y_{C:Chla_a} = \frac{0.001 K_{c_a} \Phi I_s f_c}{\mu_{MAX_a} f_{A_a}^{T1}(T) e} \quad (6.41)$$

where 0.001 is a conversion from $\mu g C$ to $mg C$, I_s is the light intensity at saturation (*Watts*), Φ is the the maximum photosynthetic quantum yield ($= 720 mg C (mol photons)^{-1}$), f_c is a conversion factor of $0.9642 mol photons m^{-2} Watt^{-1}$ and e is 2.7183. If the Webb et al. (1974) model for phytoplankton photosynthesis is to be used, then I_s can be replaced in the above expression by a value of $2.5 I_k$, based on the P-I curve approaching its upper asymptote at this value of I_k . Values of $Y_{C:Chla}$ found in nature are constrained by physiological bounds so that values determined from the above equation are also restricted to between 0.015 and 0.08.

The dynamic internal carbon model (option 4) operates similar to those for nitrogen and phosphorus. The dynamic model has the advantage of allowing the dissociation of carbon and chlorophyll-a, which may be useful in scientific applications, particularly in relation to adaptation to light and dark, or for examining storage of photosynthate product. With this model, the internal carbon is modelled as a separate state variable and operates according to 5.23 with the uptake equation defined as:

$$U_{DIC}(A_a) = UC_{MAX_a} \left[f_{A_a}^{T1}(T) \left(\frac{AIC_{MAX_a} - AIC_a}{AIC_{MAX_a} - AIC_{MIN_a}} \right) \left(\frac{I}{I_{s_a}} \exp \left(1 - \frac{I}{I_{s_a}} \right) \right) \right] A_a \quad (6.42)$$

for the photoinhibited case, where UC_{MAX} is the maximum uptake rate of carbon, AIC_{MAX} is the maximum internal carbon to chlorophyll-a ratio, AIC_{MIN} is the minimum internal carbon to chlorophyll-a ratio, and A must be in chlorophyll-a units. For the non-photoinhibited case (Webb et al., 1974):

$$U_{DIC}(A_a) = UC_{MAX_a} \left[f_{A_a}^{T1}(T) \left(\frac{AIC_{MAX_a} - AIC_a}{AIC_{MAX_a} - AIC_{MIN_a}} \right) \left(1 - \exp \left(-\frac{I}{I_{k_a}} \right) \right) \right] A_a. \quad (6.43)$$

For the respiration, mortality and excretion losses, equations 6.38 and 6.40 still apply, but with $Y_{C:Chla} = AIC/A$. Settling again applies equally to the internal carbon as to the chlorophyll-a biomass of each group, as for the other internal nutrients represented.

Note that with all but the dynamic model, the only carbon dependence for growth is that there must be sufficient DIC available if inorganic carbon is configured, otherwise carbon is assumed to be non-limiting. For the dynamic model, carbon limitation is calculated as done for the nutrients:

$$f(C)_a = \frac{AIC_{MAX_a}}{AIC_{MAX_a} - AIC_{MIN_a}} \left[1 - \frac{AIC_{MIN_a}}{AIC_a} \right]. \quad (6.44)$$

Silica: The silica model within CAEDYM allows for uptake of dissolved silica, an internal store of silica, and loss through mortality and excretion (Figure 5.5). Note that silica dynamics (and the SiO_2 state variable) are only included if the diatom species are modelled - phytoplankton groups 6 & 7 (MDIAT & FDIAT). For all other species, silica is not considered important and is therefore not modelled. For the diatom species, the silica limitation function is similar to that for nitrogen and phosphorus:

$$f(Si)_a = \frac{SiO_2 - SiO_{2o}}{(SiO_2 - SiO_{2o}) + K_{Si_a}} \quad (6.45)$$

where SiO_{2o} is minimum concentration of silica at which growth ceases, and K_{Si} is the half-saturation constant for the effect of silica on the growth rate. No dynamic model for internal silica concentrations exists within CAEDYM, so the internal silica concentration is simply the growth rate multiplied by the user-defined internal silica to chlorophyll-a ratio, k_{ISi} :

$$U_{SiO_2}(A_a) = k_{ISi_a} \mu_{g_a}. \quad (6.46)$$

During algal senescence, silica loss is considered to be particulate (i.e. the husks of the cells) and to settle directly to the sediments. The loss is modelled similar to the other nutrients:

$$E_{SiO_2}(A_a) = k_{ISi_a} L_a f(S)_a. \quad (6.47)$$

6.2.2 Respiration, Mortality & Excretion: Loss terms represented in the model include a lumped term for metabolic loss, and grazing (discussed later). The metabolic loss term, L , is a lumped parameterization of respiration, natural mortality and excretion, and takes the form:

$$L = k_{r_a} \vartheta^{T-20} \quad (6.48)$$

where k_{r_a} is the 'respiration' rate coefficient (although it also includes the effects of mortality and excretion). Values of k_r , as a fraction of production, have been established for many marine and estuarine phytoplankton by Langdon (1993) and many others. Note that CAEDYM also employs a constant, f_{RES} , that is used to isolate true respiration losses from the lumped parameterization. In addition, the constant f_{DOM} is also used to isolate the fraction of mortality and excretion that goes into the dissolved organic pool, and the fraction that enters the particulate organic pool.

Effect of salinity: The loss term is multiplied by $f(S)$, defined as the respiration response to salinity. For freshwater phytoplankton (e.g. cyanobacteria, chlorophytes and freshwater diatoms), the function takes the form:

$$f(S) = \begin{cases} 1.0 & : S \leq S_{opt} \\ \frac{(\beta-1)S^2}{(S_{max}-S_{opt})^2} - \frac{2(\beta-1)S_{opt}S}{(S_{max}-S_{opt})^2} + \frac{(\beta-1)S_{opt}^2}{(S_{max}-S_{opt})^2} + 1 & : S > S_{opt} \end{cases} \quad (6.49)$$

where β is the value of $f(S)$ when salinity is maximal (taken as 36), and S_{opt} is the salinity at which $f(S)$ is 1.0 (i.e. the minimum value of $f(S)$). This expression is parabolic, so that the effect of $f(S)$ is to increase the respiration rate as salinities increase above S_{opt} .

Changing the type of freshwater environment will allow marine phytoplankton groups to be simulated as freshwater and vice versa, without any limitation by salinity. The type of salinity environment is set via the variable *wmode* to either freshwater, marine or estuarine. Only in the case of estuarine applications is the salinity function activated if the *wmode* variable is set to an estuarine application. In addition, the flag *phsal* enables complete freedom to be able to assign the salinity preferences as appropriate for each phytoplankton group simulated, with the salinity parameters then set for each phytoplankton group. This mode of operation may be useful when, for example, there is an application involving simulation of two freshwater cyanobacterial groups or species.

For marine groups (dinoflagellates, cryptophytes and marine diatoms) the salinity response is given by:

$$\begin{aligned} f(S) &= 1.0 & : S \leq S_{opt} \\ f(S) &= \frac{(\beta-1)S^2}{S_{opt}^2} - \frac{2(\beta-1)S}{S_{opt}} & : S > S_{opt} \end{aligned} \quad (6.50)$$

where β is the value of $f(S)$ when the salinity is zero for these marine groups and S_{opt} is the salinity at which $f(S)$ is 1.0 (i.e. the minimum value of $f(S)$). This expression is a parabolic one, so that the effect of $f(S)$ is to increase the respiration rate as salinities decrease below S_{opt} (Fig. 5).

The remaining $f(S)$ term applies to Nodularia or an estuarine cyanobacterial group for example and is given by:

$$f(S) = \frac{(\beta-1)S^2}{S_{opt}^2} - \frac{2(\beta-1)S}{S_{opt}} + \beta \quad (6.51)$$

It should be noted that this expression is symmetrical about S_{opt} , with β being the value of $f(S)$ when the salinity is zero or when the salinity is $2 \times S_{opt}$ (Fig. 6).

If the application is for freshwater and the user wishes to simulate two freshwater cyanobacterial groups, then specifying a freshwater case with intention to simulate both of these groups in the parameter input file (*phsal* set to freshwater).

6.2.3 Vertical Migration, Settling & Resuspension: There are 4 models available to the user for phytoplankton migration and settling:

1. constant, user-defined settling velocity;
2. settling velocity based on stokes sedimentation kinetics;
3. migration without photoinhibition; and
4. migration with photoinhibition

Vertical migration without inhibition (intended for cyanobacteria for example) has been quantified numerically using the model of Kromkamp and Walsby (1990). This model gives the rate of change in density with time ($kg\ m^{-3}\ min^{-1}$) as:

$$\frac{d\rho}{dt} = c_1 \left[\frac{I}{I_K + I} \right] - c_3 \quad (6.52)$$

where c_1 is the rate coefficient that determines the decrease in density with time (given by Kromkamp and Walsby (1990) as $0.132\ (kg\ m^{-3}\ min^{-1})$), I is the irradiance ($\mu E\ m^{-2}\ s^{-1}$), I_K is the half saturation constant for the rate of increase in density with time (given by Kromkamp and Walsby (1990) as $25\ \mu E\ m^{-2}\ s^{-1}$), and c_3 is the minimum rate of density increase (given by Kromkamp and Walsby (1990) as $0.132\ kg\ m^{-3}\ min^{-1}$). To be consistent with the formulation used previously to describe the photosynthetic response of phytoplankton to light, the above formula is modified to include the Webb et al. (1974) formulation for the light response:

$$\frac{d\rho}{dt} = c_1 \left[1 - \exp\left(-\frac{I}{I_K}\right) \right] - c_3 \quad (6.53)$$

This change may effect small deviations in the values of c_1 and c_3 from those given by Kromkamp and Walsby (1990), necessitating some calibration of the model parameters.

If it is decided to base the change in density is dependent on the rate of accumulation of photosynthate, then the internal carbon store, IC , is used to determine density as follows:

$$\frac{d\rho}{dt} = c_2 \left[1 - \frac{AIC_{MIN}}{AIC} \right] - c_3 \quad (6.54)$$

where AIC_{MIN} is the minimum permissible internal carbon to chlorophyll-a ratio. This expression implies that the cells will migrate upward progressively more weakly as they accumulate photosynthate. Again, c_1 and c_3 may require some fine tuning in this mode.

For the case of darkness (again, for cyanobacterial cells for example), the rate of decrease of density after four hours was found by Kromkamp and Walsby (1990) to be a linear function of previous irradiance, I_a :

$$\frac{d\rho}{dt} = c_2 I_a - c_3 \quad (6.55)$$

where c_2 is the rate coefficient for light-dependent changes in density with time (given as $7.67 \times 10^{-5}\ kg\ m^{-3}\ min^{-1}\ (\mu E\ m^{-2}\ s^{-1})^{-1}$). This expression says nothing about the time dependence of density changes for periods other than four hours. Re-evaluation of the expression has resulted in assigning the rate of density change in the absence of light to a constant:

$$\frac{d\rho}{dt} = -c_3. \quad (6.56)$$

Vertical migration of dinoflagellates, chlorophytes and cryptophytes is represented numerically on the basis of the balance between irradiance and internal nitrogen stores. The model used to determine the response to light is similar to that used by Kromkamp and Walsby (1990). The migratory response to nutrients is regulated by

the internal nitrogen store in the cell and the external nitrogen supply to the cell. The combination of the two is represented for the case without photoinhibition as:

$$\frac{d\rho}{dt} = c_4 \left[1 - \exp\left(-\frac{I}{I_K}\right) \right] - c_5 \left[1 - \left(\frac{AIN - AIN_{MIN}}{AIN_{MAX} - AIN_{MIN}} \right) \right], \quad (6.57)$$

and for the case which includes photoinhibition as:

$$\frac{d\rho}{dt} = c_4 \left[\frac{I}{I_s} \exp\left(1 - \frac{I}{I_s}\right) \right] - c_5 \left[1 - \left(\frac{AIN - AIN_{MIN}}{AIN_{MAX} - AIN_{MIN}} \right) \right], \quad (6.58)$$

where c_4 is a calibrated rate coefficient for light-dependent changes in migration velocity ($m \min^{-1}$) and c_5 is a calibrated rate coefficient for nutrient-dependent changes in migration velocity ($m \min^{-1}$). The appropriate expression is activated by the user depending on which choice is made with respect to inhibition. Application of this formulation in the model involves first determining the maximum nitrogen concentration in any layer over the depth of the water column. In the rare instance in which this layer is above the layer under consideration, then the sign of c_5 is changed to negative. For the case where carbon accumulation is to be used, the velocity is determined as:

$$\frac{d\rho}{dt} = c_4 \left[1 - \frac{AIC_{MIN}}{AIC} \right] - c_5 \left[1 - \left(\frac{AIN - AIN_{MIN}}{AIN_{MAX} - AIN_{MIN}} \right) \left(\frac{NH_4 + NO_3}{K_N + NH_4 + NO_3} \right) \right], \quad (6.59)$$

In this expression the first part of the equation reduces to zero at night so that there is no upward migration at this time.

The velocities generated from the dinoflagellate, chlorophyte and cryptophyte phytoplankton models can be used to determine the vertical distance moved over each time step, and to recalculate the position of cells relative to the model layers. The calculated value of v_{A_a} is used to determine the distance migrated by the dinoflagellates, cryptophytes and chlorophytes over each time step. If this distance exceeds that required to reach the maximum light field (i.e., the water surface) or if it exceeds the distance to reach the maximum nitrogen concentrations (i.e., typically the bottom) then phytoplankton migration distances are curtailed to maintain them within the prescribed model boundaries.

For the stokes settling model cell densities are generated dynamically from the above expressions and a Stokes settling formula is invoked to determine the vertical velocities:

$$v_{A_a} = \frac{g(\rho_{A_a} - \rho_w) d_{A_a}^2}{18\mu} \quad (6.60)$$

where g is acceleration due to gravity, ρ_{A_a} is the density of phytoplankton group, a , ρ_w is the density of water, d_{A_a} is the diameter of the phytoplankton group and μ is the viscosity of water.

Where phytoplankton settle into the sediments they are assumed to live for a period of time (usually one day) in the sediments. During this period, the phytoplankton may be resuspended into the bottom layer of the water column. If the phytoplankton do not re-enter the water column, their biomass enters the respective nutrient

pools in the sediment. Resuspension is calculated as for other particles based on a critical shear stress, τ_{cA} and resuspension rate constant, α_A :

$$f_{A_a}^{RES} = \alpha_{A_a} \left[\frac{\tau - \tau_{cA_a}}{\tau_{ref}} \right] \left[\frac{A_{a_{SED}}}{\tilde{K}_{T_{A_a}} + A_{a_{SED}}} \right]; \quad (6.61)$$

more information on resuspension is provided in Section 10.2.

6.2.4 Grazing

Zooplankton: Five zooplankton groups are included in the model and are discussed in some detail in Section 6.3. There is substantial flexibility as to how these groups can be partitioned by the user.

The rate of removal of phytoplankton from the water due to grazing by these groups is determined using the following model. Each zooplankton group, z , has a grazing preference for a particular phytoplankton group a , denoted by P_{za} , P_{zz} for zooplankton grazing on other zooplankton, and for detrital material (POM), denoted by P_{zd} . The weighted grazing function, f^{ZGW} , by zooplankton group z on each of the phytoplankton groups a is therefore denoted by:

$$f_{A_a}^{ZGW}(Z_z, A_a) = \frac{P_{za} A_a Y_{C:Chla_a}}{\sum_a^{N_A} [P_{za} A_a Y_{C:Chla_a}] + \sum_k^{N_Z} [P_{zk} Z_k] + \sum_d^{N_D} [P_{zd} POC_d]} \quad (6.62)$$

where A_a is the chlorophyll-a ($\mu g Chla L^{-1}$) associated with each phytoplankton group a , Z_z is the biomass of zooplankton group z as $mg C L^{-1}$, $Y_{C:Chla}$ is the mass of carbon (mg) to chlorophyll-a (μg) in phytoplankton, N_D is the number of detrital groups. Appropriate choice of parameters in this expression (i.e. setting grazing preferences solely to phytoplankton by setting the remaining grazing preferences to zero) will limit grazing by zooplankton to phytoplankton.

The grazing function, f^{GRZ} , is used to describe the rate of removal of phytoplankton group a due to grazing by all zooplankton groups is thus:

$$f_{A_a}^{GRZ_X}(Z, 0, A_a) = \sum_z^{N_Z} G_X(Z_z) f_{A_a}^{ZGW}(Z_z, g) \quad (6.63)$$

where X is the nutrient of interest: C , N or P . The above fomula sums over each zooplankton group z in order to determine the total removal of phytoplankton group a ; $f_{A_a}^{GRZ}$ has units of $mg Chla L^{-1} day^{-1}$. For more detail on the estimation of G , see Section 6.3).

Bivalves: The rate of removal of phytoplankton from the water due to grazing by bivalves is determined similarly but only applies in the benthos (that is the water cell located immediately above the sediment). Bivalves have a grazing preference for a particular phytoplankton group a , denoted by P_{bva} , and for detrital material

(POM), denoted by P_{bvd} . The weighted grazing function, f^{BZW} , by bivalves on each of the phytoplankton groups a is therefore denoted by:

$$f_{A_a}^{BGW}(BV_b, A_a) = \frac{P_{bva} A_a Y_{C:Chla_a}}{\sum_a^{N_A} [P_{bva} A_a Y_{C:Chla_a}] + \sum_d^{N_D} [P_{bvd} POC_d]} \quad (6.64)$$

where A_a is the chlorophyll-a ($\mu g Chla L^{-1}$) associated with each phytoplankton group a , $Y_{C:Chla_a}$ is the mass of carbon (mg) to chlorophyll-a (μg) in phytoplankton, and N_D is the number of detrital groups. Appropriate choice of parameters in this expression (i.e. setting grazing preferences solely to phytoplankton by setting the remaining grazing preferences to zero) will limit grazing of bivalves solely to phytoplankton.

Therefore equation to describe the rate of removal of phytoplankton group a due to grazing by bivalves is thus:

$$f_{A_a}^{GRZX}(BV, A_a) = \frac{GBZ f(Z_{BV}) f(W)_{bvi} BV f_{BV}(T)}{\Delta z_{bot} Y_{C:Chla}} \quad (6.65)$$

where G_a^{BV} has units of $mg Chla day^{-1}$, GBZ is the grazing rate coefficient as mg phytoplankton C (mg bivalve C) $^{-1} day^{-1}$, $Y_{C:Chla}$ is the internal carbon ($mg C (mg chlorophyll - a)^{-1}$), BV is the bivalve biomass ($g C m^{-2}$) and $f(Z_{BV})$ is the Michaelis-Menten function for bivalve grazing (discussed in more detail in Section 7.4.1).

6.2.5 Algal Toxin & Metabolite Production: Each algal group can be configured to produce metabolites for applications examining taste and odour compounds or algal toxin dynamics. The water column concentration of the toxin/metabolite, X_a ($mg L^{-1}$), is estimated from:

$$\frac{\partial X_a}{\partial t} = \underbrace{f_{A_a}^{BME}}_{\text{cell lysis \& excretion}} - \underbrace{f_{X_a}^{MIN}}_{\text{microbial decay}} \quad (6.66)$$

where $f_{A_a}^{BME}$ is the metabolite contribution from mortality and excretion by A_a , and $f_{X_a}^{MIN}$ is the bacterially mediated decay of metabolites. Although the processes introduced here are similar to those described earlier, they are not described by the generic parameterizations described in Table 5.1, and are defined as:

$$f_{A_a}^{BME} = IX_a A_a (1 - f_{RES_a}) L_a f(S)_a \quad (6.67)$$

$$f_{X_a}^{MIN} = -m_X T X_a \quad (6.68)$$

where IX_a is the internal metabolite concentration of group a ($mg L^{-1} (mg Chla L^{-1})^{-1}$) and m_X is a degradation rate constant.

The metabolite concentration within the algal cells, IX_a , is considered to be a linear function of the growth rate, μ_g (see Long et al. (2001):

$$IX_a = IX_{a-min} + \frac{\mu_{g_a}}{\mu_{MAX_a}} (IX_{a-MAX} - IX_{a-MIN}) \quad (6.69)$$

where IX_{a-MIN} is the minimum internal metabolite concentration (i.e when the growth rate is zero), IX_{a-MAX} is the internal metabolite concentration during maximum production. The linear dependence can be avoided by setting the max and min parameters to be the same value.

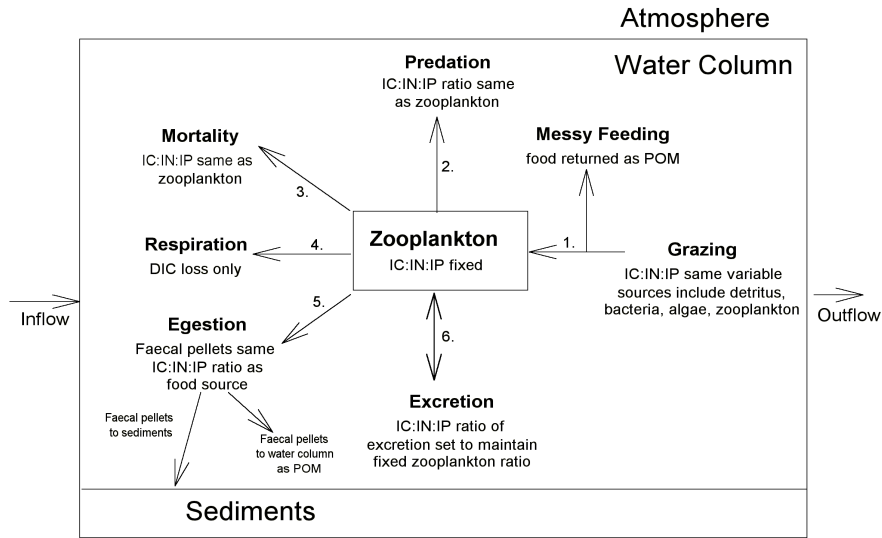


Figure 6.2 Schematic of zooplankton dynamics within CAEDYM.

6.3 Zooplankton

6.3.1 Overview: Upto five generic zooplankton groups are configurable within CAEDYM (state variables $ZOOP1 - ZOOP5$). All of these groups have the same functionality, as outlined throughout this section. Therefore the groups can be used to model several unique species, or different size classes of a single species for example. Figure 6.2 provides an overview of zooplankton dynamics as captured by CAEDYM, and mass balance equations for zooplankton carbon nitrogen and phosphorus are listed in the previous chapter. The remainder of the section outlines in detail the estimation of the process influencing zooplankton behavior.

6.3.2 Grazing: Zooplankton graze on phytoplankton (which may be simulated with or without dynamically calculated internal nutrient supplies), detritus (made up of particulate carbon, nitrogen and phosphorus, bacteria, and on other zooplankton. Grazing preferences are assigned to each food source (A , Z , $POCL$, $POCR$ & B), and the overall potential rate of carbon consumption is regulated by a Michaelis-Menten function, $f_{Z_z}^{ZFD}$ for available food supply:

$$f_{Z_z}^{ZFD}(A, Z, B, POC) = \frac{\sum_a^{N_A} A_a Y_{C:Chla_a} + \sum_k^{N_Z} Z_k + \sum_d^{N_D} POC_d + B}{K_{Z_z} + \sum_a^{N_A} A_a Y_{C:Chla_a} + \sum_k^{N_Z} Z_k + \sum_d^{N_D} POC_d + B} \quad (6.70)$$

where K_{Z_z} is the half-saturation constant for the effect of food abundance on grazing. Each zooplankton group, z , has a grazing preference for a particular phytoplankton group a , denoted by P_{za} , P_{zk} for zooplankton grazing on other zooplankton, and for detrital material (POM), denoted by P_{zd} . Therefore, we can calculate the total amount of carbon grazed, G , from:

$$G_C(Z_z) = g_{MAX_z} f_{Z_z}^{T1}(T) f_{Z_z}^{ZFD}(A, Z, B, POC) Z_z \quad (6.71)$$

where g_{MAX} is the grazing rate coefficient (mg consumed C (mg zooplankton C) $^{-1}$ day^{-1}), and $f_{Z_z}^{T1}(T)$ is a function for temperature dependence of grazing (refer to phytoplankton temperature sub-section for information on f^{T1}). Nutrient accumulation through grazing is more complicated since the sources may have different nutrient concentrations. A grazing function for nutrients is therefore requires knowledge of the relative contribution of each food source, defined using a weighting function:

$$f_Y^{ZGW}(Z_z, Y) = \frac{P_{zy}Y}{\sum_a^{N_A}[P_{za} A_a Y_{C:Chla_a}] + \sum_k^{N_Z}[P_{zk} Z_k] + \sum_d^{N_D}[P_{zd} POC_d]} \quad (6.72)$$

where y is a generic group index and Y is the substance of concern (i.e. A_a , Z_z , POC_d or B in carbon units). Using this weighting function, the nitrogen consumption is modelled as:

$$\begin{aligned} G_N(Z_z) = & \underbrace{\sum_a^{N_A} G_C(Z_z) f_{A_a}^{ZGW}(Z_z, A_a) \frac{AIN_a}{A_a} P_{za}}_{\text{a-N from phytoplankton}} + \underbrace{\sum_k^{N_Z} G_C(Z_z) f_{Z_k}^{ZGW}(Z_z, Z_k) k_{ZIN_k} P_{zk}}_{\text{a-N from zooplankton}} \\ & + \underbrace{G_C(Z_z) f_B^{ZGW}(Z_z, B) k_{BIN} P_{zb}}_{\text{a-N from bacteria}} + \underbrace{\sum_d^{N_D} G_C(Z_z) f_{POC_d}^{ZGW}(Z_z, POC_d) \frac{PON_d}{POC_d} P_{zd}}_{\text{a-N from POM}} \end{aligned} \quad (6.73)$$

where k_{ZIN_z} is the user-defined internal nitrogen concentration (mg N (mg C) $^{-1}$) of the z^{th} zooplankton being consumed and AIN_a is the internal algal N concentration (see Section 6.2). Similarly, the phosphorus intake equation is written as:

$$\begin{aligned} G_P(Z_z) = & \underbrace{\sum_a^{N_A} G_C(Z_z) f_{A_a}^{ZGW}(Z_z, A_a) \frac{AIP_a}{A_a} P_{za}}_{\text{a-P from phytoplankton}} + \underbrace{\sum_k^{N_Z} G_C(Z_z) f_{Z_k}^{ZGW}(Z_z, Z_k) k_{ZIP_k} P_{zk}}_{\text{a-P from zooplankton}} \\ & + \underbrace{G_C(Z_z) f_B^{ZGW}(Z_z, B) k_{BIP} P_{zb}}_{\text{a-P from bacteria}} + \underbrace{\sum_d^{N_D} G_C(Z_z) f_{POC_d}^{ZGW}(Z_z, POC_d) \frac{POP_d}{POC_d} P_{zd}}_{\text{a-P from POM}} \end{aligned} \quad (6.74)$$

where k_{ZIP_z} is the user-defined internal phosphorus concentration (mg P (mg C) $^{-1}$) for the z^{th} zooplankton being consumed and AIP_a is the internal algal P concentration (see Section 6.2).

6.3.3 Predation: It is assumed in the model that consumption by fish is a major zooplankton loss from the water column. To model fish grazing, a weighted preference is first assigned to each zooplankton group:

$$f_{Z_z}^{FGW}(F_f, Z_z) = \frac{P_{fz} Z_z}{\sum_a^{N_A}[P_{fa} A_a Y_{C:Chla_a}] + \sum_k^{N_Z}[P_{fk} Z_k] + \sum_d^{N_D}[P_{fd} POC_d]} \quad (6.75)$$

where P_{fz} is the preference of fish group f on zooplankton group z relative to the total composition of their diet.

For grazing by other zooplankton, a weighted preference is allocated to each zooplankton group according to 6.72.

Therefore the total loss of zooplankton through grazing by fish and other zooplankton is given by:

$$f_{Z_z}^{GRZX}(Z, F, Z_z) = \sum_k^{N_Z} G_X(Z_z) f_{Z_z}^{ZGW}(Z_z, Z_k) + \sum_f^{N_F} G_X(F_f) f_{Z_z}^{FGW}(F_f, Z_z) \quad (6.76)$$

where X is the nutrient of interest: C , N or P . The above formula sums over each zooplankton group k , and each fish group, f , in order to determine the total removal of zooplankton group z . For more detail on the estimation of G by the fish, see Section 6.4).

6.3.4 Respiration: Respiration is modelled by using a respiration rate coefficient, k_{zR_z} for each zooplankton class, z , and assigning the usual temperature dependence:

$$R_{DIC}(Z_z) = k_{zR_z} \vartheta^{T-20} Z_z. \quad (6.77)$$

The carbon lost to CO_2 is used to increment the DIC concentration if DIC is being simulated, and the equivalent mass of O_2 is also consumed. No nutrients are lost through respiration.

6.3.5 Mortality, Excretion & Egestion: Zooplankton losses through mortality, excretion and egestion (i.e. faecal pellets) are modelled according to:

$$E_{DOCL}(Z_z) = \underbrace{k_{zE_z} G_C(Z_z)}_{\text{excretion}} \quad (6.78)$$

$$E_{POCL}(Z_z) = \underbrace{k_{zF_z} G_C(Z_z)}_{\text{faecal pellets}} + \underbrace{k_{zM_z} \vartheta^{T-20} Z_z}_{\text{mortality}} \quad (6.79)$$

where k_{zE_z} and k_{zF_z} are fractions of the grazed food that are lost to excretion and faecal pellets respectively, and k_{zM_z} is the mortality rate coefficient (day^{-1}).

The nutrient loss due to mortality contributes to (labile) particulate N and P , and because zooplankton internal nutrient ratios are fixed, the nutrient loss due to mortality is expressed as the amount of carbon lost to mortality multiplied by the zooplankton internal nutrient concentration (k_{ZIN_z} and k_{ZIP_z}). For nutrient loss via faecal pellets, the nutrient concentration is assumed not be the zooplankton internal nutrient concentration, but the mean nutrient concentration of all the grazed food. Therefore, the loss of nutrients from the zooplankton pool to particulate detritus is calculated from:

$$E_{PONL}(Z_z) = \underbrace{k_{zF_z} G_N(Z_z)}_{\text{faecal pellets}} + \underbrace{k_{zM_z} \vartheta^{T-20} k_{ZIN_z} Z_z}_{\text{mortality}} \quad (6.80)$$

for nitrogen, and:

$$E_{POPL}(Z_z) = \underbrace{k_{zF_z} G_P(Z_z)}_{\text{faecal pellets}} + \underbrace{k_{zM_z} \vartheta^{T-20} k_{ZIP_z} Z_z}_{\text{mortality}} \quad (6.81)$$

for phosphorus. The loss of nutrients via excretion to the dissolved organic pool however, is more complicated as this term is used to maintain the user-defined constant internal nutrient ratio within the zooplankton. Therefore, each of the processes described above are performed first and stored in an auxiliary/buffer(*) array, and then any excess N or P is removed. In the case of a nutrient limited system, excess carbon must also be removed. There are

therefore 4 possible scenarios: both N and P are in excess, P is limiting, N is limiting or both N and P is limiting. For the first case it is simply a matter of removing the excess nutrients to maintain the internal ratio:

$$E_{DONL}(Z_z) = \frac{ZIN_z^* - Z_z^{t+1} k_{ZIN_z}}{\Delta t} \quad (6.82)$$

for nitrogen, and:

$$E_{DOPL}(Z_z) = \frac{ZIP_z^* - Z_z^{t+1} k_{ZIP_z}}{\Delta t} \quad (6.83)$$

for phosphorus, where ZIN and ZIP are concentrations of zooplankton internal nitrogen and phosphorus respectively, the * indicates that value has already been update by grazing, mortality and egestion, Z_z^{t+1} is the zooplankton concentration at the forward timestep (i.e. after it has been updated with the carbon fluxes previously described in this section). For the case where phosphorus is limiting (i.e. insufficient phosphorus uptake to maintain internal homeostasis), then some extra carbon must be excreted (as $DOCL$). The nitrogen excreted is then same as for 6.82, but using the incremented carbon concentration, and $E_{DOPL} = 0$. For the case where nitrogen is limiting (i.e. insufficient nitrogen uptake to maintain internal homeostasis), then some extra carbon must be excreted (as $DOCL$). The phosphorus excreted is then same as for 6.83, but using the incremented carbon concentration, and $E_{DONL} = 0$. If both N and P are limiting, $DOCL$ is excreted until the k_{ZIN} and k_{ZIP} are satisfied.

6.4 Fish

6.4.1 Overview: Upto three generic fish groups are configurable within CAEDYM (state variables $FISH1$ – $FISH3$). All of these groups have similar functionality, although, unlike zooplankton, fish are capable of recruiting from different fish classes. Therefore the groups can be used to model several unique species, or different size/age classes of a single species can be explicitly modelled. Figure 6.3 provides an overview of fish dynamics as captured by CAEDYM, and balance equations for fish C , N and P are presented in Chapter 5. The remainder of the section outlines in detail the estimation of the process influencing fish behavior.

6.4.2 Grazing: Fish can potentially graze on phytoplankton (which may be simulated with or without internal nutrient supplies), detritus (made up of particulate carbon, nitrogen and phosphorus), on zooplankton, other fish, on benthic macroinvertebrates and macroalgae and macrophytes. Grazing preferences are assigned to each food source (A , Z , POC , F , BV , GZ , PC , M and SG), and the overall potential rate of carbon consumption is regulated by a Michaelis-Menten function, $f_{F_f}^{FFD}$ for available food supply:

$$f_{F_f}^{FFD}(A, Z, POC, F, BV, GZ, PC, M, SG) = \frac{\sum_a^{N_A} A_a Y_{C:Chla_a} + \sum_k^{N_Z} Z_k + \sum_d^{N_D} POC_d + \sum_f^{N_f} F_f + \sum_m^{N_M} M_m + SG + BV + GZ + PC}{K_{F_f} + \sum_a^{N_A} A_a Y_{C:Chla_a} + \sum_k^{N_Z} Z_k + \sum_d^{N_D} POC_d + \sum_f^{N_f} F_f + \sum_m^{N_M} M_m + SG + BV + GZ + PC} \quad (6.84)$$

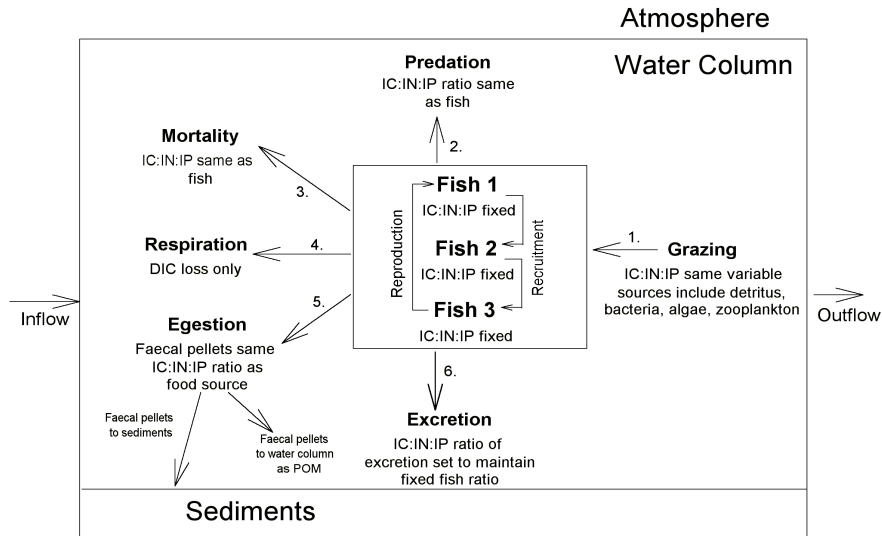


Figure 6.3 Schematic of fish dynamics within CAEDYM.

where K_{F_f} is the half-saturation constant for the effect of food abundance on grazing. Each fish group, f , has a grazing preference for a particular phytoplankton group a , denoted by P_{fa} , P_{fz} for fish grazing on zooplankton, P_{ff} for fish grazing on other fish, P_{fbv} for fish grazing on bivalves, P_{fpc} for fish grazing on polychaetes, P_{fgz} for fish grazing on crustaceans, P_{fm} for fish grazing on macroalgae, P_{fs} for fish grazing on seagrasses/macrophytes, and P_{fd} for fish grazing on detrital material (POM). Therefore, we can calculate the total amount of carbon grazed, denoted $f_{F_f}^{GRZC}$, for each fish group from:

$$G_C(F_f) = g_{MAX_f} f_{F_f}^{T1}(T) f_{F_f}^{FFD}(A, Z, POC, F, BV, GZ, PC, M, SG) F_f \quad (6.85)$$

where g_{MAX} is the grazing rate coefficient (mg consumed C (mg fish C) $^{-1}$ day^{-1}), and $f_{F_f}^{T1}(T)$ is a function for temperature dependence of grazing (refer to phytoplankton temperature sub-section for information on f^{T1}). Nutrient accumulation through grazing is more complicated since the sources may have different nutrient concentrations. A grazing function for nutrients therefore requires knowledge of the relative contribution of each food source, defined using a weighting function:

$$f_Y^{FGW}(F_f, Y) = P_{fy} Y \left\{ \sum_a^{N_A} [P_{fa} A_a Y_{C:Chla_a}] + \sum_z^{N_Z} [P_{fz} Z_z] + \sum_d^{N_D} [P_{fd} POC_d] \right. \\ \left. + \sum_k^{N_F} [P_{fk} F_k] + \sum_m^{N_M} [P_{fm} M_m] + P_{fs} SG + P_{fbv} BV + P_{fpc} PC + P_{fgz} GZ \right\}^{-1} \quad (6.86)$$

where y is a generic group index and Y is the substance of concern (i.e. A_a , Z_z , POC_d , F_f etc. in carbon units).

Using this weighting function, the nitrogen consumption is modelled as:

$$\begin{aligned}
G_N(F_f) = & \underbrace{\sum_a^{N_A} G_C(F_f) f_{A_a}^{FGW}(F_f, A_a) \frac{AIN_a}{A_a} P_{fa}}_{\text{a-N from phytoplankton}} + \underbrace{\sum_z^{N_Z} G_C(F_f) f_{Z_z}^{FGW}(F_f, Z_z) k_{ZIN_z} P_{fz}}_{\text{b-N from zooplankton}} \\
& + \underbrace{\sum_d^{N_D} G_C(F_f) f_{POC_d}^{FGW}(F_f, POC_d) \frac{PON_d}{POC_d} P_{fd}}_{\text{c-N from POM}} + \underbrace{\sum_k^{N_F} G_C(F_f) f_{F_k}^{FGW}(F_f, F_f) k_{FIN_k} P_{fk}}_{\text{d-N from fish}} \\
& + \underbrace{G_C(F_f) f_{BV}^{FGW}(F_f, BV) k_{BVIN} P_{fbv}}_{\text{e-N from bivalves}} + \underbrace{G_C(F_f) f_{GZ}^{FGW}(F_f, GZ) k_{GZIN} P_{fgz}}_{\text{f-N from crustaceans}} \\
& + \underbrace{G_C(F_f) f_{PC}^{FGW}(F_f, PC) k_{PCIN} P_{fpc}}_{\text{g-N from polychaetes}} + \underbrace{G_C(F_f) f_{SG}^{FGW}(F_f, SG) k_{SGIN} P_{fsg}}_{\text{h-N from seagrasses}} \\
& + \underbrace{\sum_m^{N_M} G_C(F_f) f_{M_m}^{FGW}(F_f, M_m) \frac{MIN_m}{M_m} P_{fm}}_{\text{i-N from macroalgae}} \tag{6.87}
\end{aligned}$$

where k_{ZIN} , k_{FIN} , k_{BVIN} , k_{PCIN} and k_{GZIN} is the user-defined internal nitrogen concentration for zooplankton, fish, bivalves, polychaetes, and crustaceans respectively ($mg\ N\ (mg\ C)^{-1}$). Similarly, the phosphorus intake equation is written as:

$$\begin{aligned}
G_P(F_f) = & \underbrace{\sum_a^{N_A} G_C(F_f) f_{A_a}^{FGW}(F_f, A_a) \frac{AIP_a}{A_a} P_{fa}}_{\text{a-P from phytoplankton}} + \underbrace{\sum_z^{N_Z} G_C(F_f) f_{Z_z}^{FGW}(F_f, Z_z) k_{ZIP_z} P_{fz}}_{\text{b-P from zooplankton}} \\
& + \underbrace{\sum_d^{N_D} G_C(F_f) f_{POC_d}^{FGW}(F_f, POC_d) \frac{POP_d}{POC_d} P_{fd}}_{\text{c-P from POM}} + \underbrace{\sum_k^{N_F} G_C(F_f) f_{F_k}^{FGW}(F_f, F_f) k_{FIP_k} P_{fk}}_{\text{d-P from fish}} \\
& + \underbrace{G_C(F_f) f_{BV}^{FGW}(F_f, BV) k_{BVIP} P_{fbv}}_{\text{e-P from bivalves}} + \underbrace{G_C(F_f) f_{GZ}^{FGW}(F_f, GZ) k_{GZIP} P_{fgz}}_{\text{f-P from crustaceans}} \\
& + \underbrace{G_C(F_f) f_{PC}^{FGW}(F_f, PC) k_{PCIP} P_{fpc}}_{\text{g-P from polychaetes}} + \underbrace{G_C(F_f) f_{SG}^{FGW}(F_f, SG) k_{SGIP} P_{fsg}}_{\text{h-P from seagrasses}} \\
& + \underbrace{\sum_m^{N_M} G_C(F_f) f_{M_m}^{FGW}(F_f, M_m) \frac{MIP_m}{M_m} P_{fm}}_{\text{i-P from macroalgae}} \tag{6.88}
\end{aligned}$$

where k_{ZIP} , k_{FIP} , k_{BVIP} , k_{PCIP} and k_{GZIP} is the user-defined internal phosphorus concentration for zooplankton, fish, bivalves, polychaetes, and crustaceans respectively ($mg\ P\ (mg\ C)^{-1}$).

6.4.3 Predation: The model allows predation by birds and by other fish groups. Anthropogenic losses (i.e. fishing) are not currently modelled although the predation function here could be modified to include this.

The function $f_f(K)$ is used to quantify the degree to which the loss term is enhanced due to light exposure of fish. This term may be particularly important for fish which, because of unfavourable oxygen concentrations or salinities, may have to migrate into an illuminated zone where they would be at far greater risk of predation from

birds. This term is represented as:

$$f_f(K) = 1 - \frac{I_k}{I + I_k} \quad (6.89)$$

where I_k determines the way that predation is enhanced according to the available light.

For grazing by other fish, a weighted preference is allocated to each fish group according to 6.86. The loss of fish through grazing by other fish is given by:

$$f_{F_f}^{GRZX}(0, F, F_f) = \sum_k^{N_F} G_X(F_f) f_{F_f}^{FGW}(F_f, F_k). \quad (6.90)$$

The total predatory loss is the sum of that be other fish and by birds.

6.4.4 Respiration: Respiration is modelled by using a respiration rate coefficient, k_{fR_f} for each fish class, f , and assigning the usual temperature dependence:

$$R_{DIC}(F_f) = k_{fR_f} \vartheta^{T-20} F_f. \quad (6.91)$$

The carbon lost to CO_2 is used to increment the DIC concentration if DIC is being simulated, and the equivalent mass of O_2 is also consumed. No N or P is lost through respiration.

6.4.5 Mortality, Excretion & Egestion: Fish losses through mortality, excretion and egestion (i.e. faecal material) are modelled according to:

$$E_{DOCL}(F_f) = \underbrace{k_{fE_f} G_C(F_f)}_{\text{excretion}} \quad (6.92)$$

$$E_{POCL}(F_f) = \underbrace{k_{fF_f} G_C(F_f)}_{\text{faecal pellets}} + \underbrace{k_{fM_f} \vartheta^{T-20} F_f [1 + f_f^{DO1}(DO)] f(S)_f}_{\text{mortality}} \quad (6.93)$$

where k_{fE_f} and k_{fF_f} are fractions of the grazed food that are lost to excretion and faecal pellets respectively, and k_{fM_f} is the mortality rate coefficient (day^{-1}). Mortality is enhanced by a dissolved oxygen sensitivity where K_{DO_f} is the oxygen dependency for group f . This function operates above a minimum DO threshold supplied by the user; below this value the function returns 2.0, and at high DO it will return 1.0 (i.e. no mortality enhancement). Salinity also effects mortality via a salinity function $f(S)_f$:

$$f(S)_f = \quad (6.94)$$

The nutrient loss due to mortality contributes to (labile) particulate N and P, and because zooplankton internal nutrient ratios are fixed, the nutrient loss due to mortality is expressed as the amount of carbon lost to mortality multiplied by the fish internal nutrient concentration (k_{INF_f} and k_{IPF_f}). For nutrient loss via faecal material, the nutrient concentration is assumed not be the fish internal nutrient concentration, but the mean nutrient concentration of all the grazed food. Therefore, the loss of nutrients from the fish pool to particulate detritus is

calculated from:

$$E_{PONL}(F_f) = \underbrace{k_{fF_f} G_N(F_f)}_{\text{faecal pellets}} + \underbrace{k_{fM_f} \vartheta^{T-20} k_{FIN_f} F_f [1 + f_f^{DO1}(DO)] f(S)_f}_{\text{mortality}} \quad (6.95)$$

for nitrogen, and:

$$E_{POPL}(F_f) = \underbrace{k_{fF_f} G_P(F_f)}_{\text{faecal pellets}} + \underbrace{k_{fM_f} \vartheta^{T-20} k_{FIP_f} F_f [1 + f_f^{DO1}(DO)] f(S)_f}_{\text{mortality}} \quad (6.96)$$

for phosphorus. The loss of nutrients via excretion to the dissolved organic pool however, is more complicated as this term is used to maintain the user-defined constant internal nutrient ratio within the fish species. Therefore, each of the processes described above are performed first and stored in an auxiliary/buffer(*) array, and then any excess N or P is removed. In the case of a nutrient limited system, excess carbon must also be removed. There are therefore 4 possible scenarios: both N and P are in excess, P is limiting, N is limiting or both N and P is limiting. For the first case it is simply a matter of removing the excess nutrients to maintain the internal ratio:

$$E_{DONL}(F_f) = \frac{FIN_f^* - F_f^{t+1} k_{FIN_f}}{\Delta t} \quad (6.97)$$

for nitrogen, and:

$$E_{DOPL}(F_f) = \frac{FIP_f^* - F_f^{t+1} k_{FIP_f}}{\Delta t} \quad (6.98)$$

for phosphorus, where FIN and FIP are concentrations of fish internal nitrogen and phosphorus respectively, the * indicates that value has already been update by grazing, mortality and egestion, F_f^{t+1} is the fish concentration at the forward timestep (i.e. after it has been updated with the carbon fluxes previously described in this section). For the case where phosphorus is limiting (i.e. insufficient phosphorus uptake to maintain internal homeostasis), then some extra carbon must be excreted (as $DOCL$). The nitrogen excreted is then same as for 6.97, but using the incremented carbon concentration, and $E_{DOPL} = 0$. For the case where nitrogen is limiting (i.e. insufficient nitrogen uptake to maintain internal homeostasis), then some extra carbon must be excreted (as $DOCL$). The phosphorus excreted is then same as for 6.98, but using the incremented carbon concentration, and $E_{DONL} = 0$. If both N and P are limiting, $DOCL$ is excreted until the k_{FIN} and k_{FIP} are satisfied.

6.4.6 Recruitment & Spawning: The three available fish groups within CAEDYM can be used as unique species with no interaction with the other groups (aside from possible predation), or it can be used to model three size/age classes of a single species. If the latter is the intended application then transfer from one size/age class to the next is included through the adoption of ‘recruitment’ functions. CAEDYM allows users to specify unique grazing and loss rates for each size class so that older fish can have a higher mortality rate for example. In addition, the fish model includes a spawning function that allows carbon in older fish to be reallocated into juveniles.

The recruitment function currently adopted within CAEDYM employs a simple transfer equation, however, increased functionality may be added as experience develops. The transfer function from F_1 to F_2 (i.e. smallest to medium) is denoted $f_{F_2}^{REC}$ and is calculated according to:

$$f_{F_2}^{REC} = k_{1 \rightarrow 2} F_1 \quad (6.99)$$

where $k_{1 \rightarrow 2}$ is a user-defined transfer rate (day^{-1}). Similarly, F_3 recruits from F_2 :

$$f_{F_3}^{REC} = k_{2 \rightarrow 3} F_2. \quad (6.100)$$

The recruitment function for the first group is zero, $f_{F_4}^{REC} = 0$.

Reproduction by older fish is simulated by redistributing some of the older/larger fish biomass (i.e. F_3) into the smallest class (F_1). Note however, that as fish only spawn during particular periods of the year, the user must also specify a begin and end julian day (JD) for spawning to occur. Therefore the spawning function takes the form:

$$f_{F_1}^{REP} = s_e k_{3 \rightarrow 1} F_3 \quad (6.101)$$

$$f_{F_2}^{REP} = 0 \quad (6.102)$$

$$f_{F_3}^{REP} = -k_{3 \rightarrow 1} F_3 \quad (6.103)$$

for $JD_1 \leq t \leq JD_2$, where s_e is the spawning efficiency (note that $(1 - s_e) k_{3 \rightarrow 1} F_3$ is returned to the water column detrital pool), and $k_{3 \rightarrow 1}$ is the reproduction rate (day^{-1}).

If it is intended for the fish classes to not interact, then the constants $k_{1 \rightarrow 2}$, $k_{2 \rightarrow 3}$ and $k_{3 \rightarrow 1}$ must be set to zero.

6.4.7 Fish Numbers: It is often the case that not only fish biomass, but also fish size is of interest. For example, many small fish are of less interest to fishermen than a few large fish. CAEDYM therefore instansiates a ‘fish number’ state variable with each fish state variable ($NFSH1 - NFSH3$) that records the number of fish in each group. The number of fish starts based on the initial condition and then is updated at each timestep based on recruitment, spawning and losses due to mortality and predation. All other process have no effect on fish numbers, only fish biomass. The evolution of fish numbers is simply updated proportionally based on the relevant carbon transfer, e.g. if 25% of fish biomass is loss to mortality, then the number will also decrease by 25%. For the case of spawning however, fish biomass is taken from the large class and then placed in the smaller class. The user must therefore provide a parameter, denoted the ‘fishlet density’ ($number\ fish\ (g\ spawned\ C)^{-1}$), that converts reproductive carbon into number of offspring.

6.5 Jellyfish

The CAEDYM jellyfish model was developed for the Swan River in Western Australia. This state variable could potentially be adjusted to be another species of jellyfish or even another member of the planktonic community in another application.

The following description applies specifically to the Swan River. The two species of Scyphozoan medusae in the estuary are *Aurelia* sp. and *Phyllorhiza punctata*. These species are quite different in their ecology. *Phyllorhiza* occurs in the Swan River from early summer to late autumn and lives in a symbiotic relationship with the unicellular dinoflagellate *Symbiodinium* sp. *Aurelia* is a predator-grazer and primarily exerts a 'top-down' predation effect on zooplankton and larval fish. *Aurelia* is far less abundant than *Phyllorhiza* and, as there are difficulties with accurately quantifying its ecological effects and abundance, it is not included in the CAEDYM model.

For *Phyllorhiza* also, relatively little is known about its physiology, which necessitates making a number of assumptions when attempting a numerical model of its abundance and response to the prevailing environmental conditions.

It is reasonably well established that *Phyllorhiza* is only prevalent when the salinity exceeds 25ppt and also when temperatures are greater than 20°C. The numerical representation below assumes that there is equal weighting between nutrition, which is acquired through the water column in the form of organic material, and that which is derived from the symbiotic alga. Change in biomass can therefore be represented as:

$$\frac{\partial J}{\partial t} = GJ_{max} f_J(S) f_J(T) \frac{f(O) + F(L)}{2} - k_{rj} f_J(T) J - k_{ej} f_J(T) J \quad (6.104)$$

where: J is the jellyfish biomass as mL medusae m^{-3} (note that the chlorophyll content of the medusae is not explicitly represented and that the medusae are over 99% water), and GJ_{max} is the maximum relative growth rate (day^{-1}). $f_J(S)$ is a factor to regulate the response to salinity as follows:

$$\begin{aligned} f(S) &= 0 \text{ for } S \leq 25ppt \\ f(S) &= \frac{S - 25}{(K - 25) + (S - 25)} \text{ for } S > 25ppt \end{aligned} \quad (6.105)$$

where K is a rate constant. The temperature function is $f_J(T) = J^{T-25}$ (note that the usual 'T - 20' term has been replaced by 'T - 25' so that greater limitation of growth is invoked for lower temperatures. Limitation of growth by high temperatures is not expected to occur in the Swan River, particularly as high temperatures would be more likely to be associated with salinities that are lower than the usual jellyfish temperature range (i.e. well upstream in the estuary). The function $f(O)$ represents the intake of organic material from the water column:

$$f(O) = \frac{POC}{K_{POC} + POC} \quad (6.106)$$

where POC is the organic material and K_{POC} is the half-saturation constant for nutrition derived from organic material. $F(L)$ represents the nutrition of the medusae derived from the symbiotic algae, which in this case is assumed to be related solely to the light received by the jellyfish:

$$F(L) = 1 - e^{-I/I_K} \quad (6.107)$$

where I_K is the parameter controlling the response to the light climate. Finally, k_r is the respiration rate constant and k_e is the excretion rate constant.

The sum of these terms can be derived indirectly from the change in BOD of the medusae-exposed water against controls (see Rippingale, 1996), with a stoichiometric factor used to convert the BOD to carbon (and hence to biomass) for comparison against the total biomass of the medusae.

Motility, of course, greatly increases the complexity of attempts to model the jellyfish biomass. The factors governing motility are not well understood at the present point in time. A preliminary model of motility is used in CAEDYM where the medusae are assigned with an excess density over water from which the settling velocity can be determined from Stokes' Law (although it should be noted that the medusae are close to iostonic with seawater, Rippingale, 1996). Counterbalancing the downward settling velocity will be an upward swimming velocity (v_u) which depends on the light exposure as follows:

$$v_u = k \left(1 - e^{-I/I_K} \right) \quad (6.108)$$

where k is a calibratable constant (ms^{-1}). The calculated v_u is then added to the downward settling velocity, with provision that jellyfish cannot settle below or rise above the vertical water confines in the model. Note that horizontal movement is not included in the formulation and that the energy requirements of motility are also not considered. Finally, it should also be noted that mortality of jellyfish, through being washed up on beaches, has not been included.

Biological Variables (Benthic)

7.1 Introduction

CAEDYM allows for the configuration of several groups of ‘benthic’ biology:

1. 0-4 macroalgae groups (Section 7.2);
2. 0-1 seagrass/macrophyte groups (Section 7.3);
3. 0-3 macro-invertebrate groups (Section 7.4);
4. 0-3 Clam/Mussel groups (Section 7.5);

Benthic biology only operates in the cell/layer that is adjacent to the sediment and so all the functionality described within this chapter only refers to these cells. The state equations for each of these groups of variables are presented in Table 7.1. Each of processes depicted in the table and figure are discussed throughout the chapter.

Table 7.1 Summary table of equations for the benthic biological groups configurable within CAEDYM. M is the total macroalgal biomass ($mg C m^{-2}$), SG is the total seagrass/macrophyte biomass ($mg C m^{-2}$), INV is the total macroinvertebrate biomass ($mg C m^{-2}$) and CLM is the total Clam/Mussel biomass.

$$\frac{\partial M_j}{\partial t} = \underbrace{U_{DIC}(M_j)}_{\text{photosynthesis}} - \underbrace{R_{DIC}(M_j)}_{\text{respiration}} - \underbrace{E_{DOCL}(M_j) - E_{POCL}(M_j)}_{\text{mortality \& excretion}} - \underbrace{G_j}_{\text{grazing}} \quad (7.1)$$

$$\frac{\partial SG}{\partial t} = \underbrace{U_{DIC}(SG)}_{\text{photosynthesis}} - \underbrace{R_{DIC}(SG)}_{\text{respiration}} - \underbrace{E_{POCL}(SG)}_{\text{mortality \& excretion}} \quad (7.2)$$

$$\frac{\partial INV}{\partial t} = \underbrace{f_{INV}^{GRZC}}_{\text{grazing}} - \underbrace{R_{DIC}(INV)}_{\text{respiration}} - \underbrace{E_{POCL}(INV)}_{\text{mort/excr}} - \underbrace{G_{INV}}_{\text{predation}} \quad (7.3)$$

$$\frac{\partial CLM}{\partial t} = \underbrace{f_{CLM}^{GRZC}}_{\text{grazing}} - \underbrace{R_{DIC}(CLM)}_{\text{respiration}} - \underbrace{E_{POCL}(CLM)}_{\text{mort/excr}} - \underbrace{G_{CLM}}_{\text{predation}} \quad (7.4)$$

7.2 Macroalgae

Macroalgal biomass, M , is quantified on an areal basis as $g C m^{-2}$ of sediment. Four macroalgal groups can be configured within the model. As an example, in the Swan River estuarine system, *Gracillaria*, *Cystosira*, *Chaetomorpha* and *Ulva* (membranous, tubular and attached to hard substrates) are represented.

7.2.1 Growth The maximum potential growth rate is multiplied by the minimum value of expressions for limitation by light, phosphorus and nitrogen. While there may be some interaction between limiting factors, a

minimum expression is likely to provide a realistic representation of growth limitation over the relatively small spatial and temporal scales that are used for the macroalgae simulations (Rhee and Gotham, 1981).

The growth rate or gross production, μ_{g_M} (day^{-1}) can be represented as:

$$\mu_{g_M} = \mu_{max_j} \min [f(I), f(N), f(P)] f_{M_j}(T) \quad (7.5)$$

where $f(I)$, $f(N)$ and $f(P)$ represent limitation by light, nitrogen and phosphorus respectively, $f_{M_j}(T)$ is a temperature function and μ_{max} is the maximum growth rate.

Light: There are several different models for quantifying the effects of light limitation of macroalgae. Presuming that macroalgae are not photoinhibited, then the Webb et al. (1974) model can be used to quantify light dependence:

$$f(I) = 1 - \exp \left[-\frac{I}{I_k} \right] \quad (7.6)$$

where I is the photosynthetically active radiation (PAR) integrated over the depth of the bottom-most layer to the height of the macroalgae bed, and I_k is a parameter that controls the initial slope of the photosynthesis-irradiance curve.

The value of light reaching the top of the bottom layer is determined following:

$$I(1) = I(2) \exp(-K_d \Delta z) \quad (7.7)$$

where $I(1)$ is the PAR at the top of the bottom layer as a mean for each hour, $I(2)$ is the PAR at the top of the second layer as a mean for each hour, Δz is the grid cell depth and K_d is the attenuation coefficient, arrived at as:

$$\begin{aligned} K_d &= K_w (\text{attenuation due to pure water - constant}) \\ &+ \sum_i^{nphy} K_{A_i} \text{specific attenuation due to phytoplankton groups} \\ &+ \sum_b^{ndom} K_{DOC_b} \text{specific attenuation due to dissolved organic carbon} \\ &+ \sum_b^{npom} K_{POC_b} \text{specific attenuation due to particulate organic matter} \\ &+ \sum_s^{nsol} K_{SS_s} \text{specific attenuation due to inorganic particles} \\ &+ \sum_j^{nmac} K_{M_j} \text{specific attenuation due to macroalgae} \end{aligned} \quad (7.8)$$

The next step is to determine the height (h) of macroalgae in the water column, which is simply a linear function of the biomass of each group:

$$h_{mac} = \sum_j^{nmac} k_j M_j \quad (7.9)$$

here k_j is a coefficient for each of the four macroalgae groups, with units of $m\ g^{-1}$. Once the height in the water column of the macroalgal bed (h_{mac}) has been determined, the light reaching the top of the macroalgal bed, $I(mb)$ is determined as:

$$I(mb) = I(1) \exp[-K_d(z - h)] \quad (7.10)$$

where again, $I(1)$ is the light reaching the top of the bottom-most layer.

The next step is to determine the value of $f(I)$ integrated over the macroalgae bed depth and based on the integrated light for the time step duration (all using the Webb function).

Temperature: Temperature dependence is modelled as for phytoplankton (Section 6.2.1).

Nutrients: Macroalgae have compulsory internal nutrient state variables for nitrogen and phosphorous, MIN and MIP respectively. The uptake functions are modelled similar to the dynamic internal nutrient model for phytoplankton. For nitrogen:

$$U_{NO_3}(M_j) = (1 - P_{N_j}) UN_{max_j} \left[f_{M_j} \frac{MIN_{max} - MIN}{MIN_{max} - MIN_{min}} \frac{NO_3 + NH_4}{K_{N_j} + NO_3 + NH_4} \right] M_j \quad (7.11)$$

$$U_{NH_4}(M_j) = P_{N_j} UN_{max_j} \left[f_{M_j} \frac{MIN_{max} - MIN}{MIN_{max} - MIN_{min}} \frac{NO_3 + NH_4}{K_{N_j} + NO_3 + NH_4} \right] M_j \quad (7.12)$$

where P_{N_j} is the preference of group j for NH_4 as defined in equation 6.17, UN_{max_j} is the maximum uptake rate of inorganic nitrogen ($g\ N\ (g\ C)^{-1}\ day^{-1}$), and MIN_{max} and MIN_{min} are maximum and minimum values of macroalgal internal nitrogen. For phosphorous:

$$U_{PO_4}(M_j) = UP_{max_j} \left[f_{M_j} \frac{MIP_{max} - MIP}{MIP_{max} - MIP_{min}} \frac{PO_4}{K_{P_j} + PO_4} \right] M_j \quad (7.13)$$

$$(7.14)$$

where UP_{max_j} is the maximum uptake rate of inorganic phosphorous ($g\ P\ (g\ C)^{-1}\ day^{-1}$), and MIP_{max} and MIP_{min} are maximum and minimum values of macroalgal internal phosphorous.

The nutrient dependences in growth equation are calculated based on the internal nutrient concentrations:

$$f(N) = \frac{MIN_{max}}{MIN_{max} - MIN_{min}} \left[1 - \frac{MIN_{min}}{MIN} \right] \quad (7.15)$$

$$f(P) = \frac{MIP_{max}}{MIP_{max} - MIP_{min}} \left[1 - \frac{MIP_{min}}{MIP} \right]. \quad (7.16)$$

7.2.2 Respiration, Mortality, Excretion & Beach Wrack: Loss terms represented in the macroalgae model include a lumped (salinity dependent) metabolic loss term (respiration, mortality and excretion), loss as

beach wrack, and loss through grazing (discussed in the next section). The lumped metabolic loss for macroalgal group j , L_j , is modelled as:

$$L_j = k_{rM_j} \vartheta^{T-20} f_{M_j}(S) \quad (7.17)$$

where k_{rM_j} is the ‘respiration’ rate coefficient and $f_{M_j}(S)$ is a response of respiration to salinity, as given by:

$$f_{M_j}(S) = \frac{\beta - 1}{S_{opt}^2} S^2 - \frac{2(\beta - 1)}{S_{opt}} S + \beta \quad (7.18)$$

This expression is a parabolic one, so that the effect of $f_{M_j}(S)$ is to increase the respiration rate as salinities increase above and decrease below S_{opt} . Here the value of β is set to 2.0.

Using these expressions, the respiration and biological mortality and excretion functions (equations 5.15 and 5.13) for macroalgae are:

$$R_{DIC}(M_j) = f_{resM_j} L_j \frac{M_j}{\Delta z_{bot}} \quad (7.19)$$

$$E_{POCL}(M_j) = (1 - f_{resM_j}) L_j \frac{M_j}{\Delta z_{bot}} + E_{POCL}^{BW}(M_j) \quad (7.20)$$

$$E_{NH_4}(M_j) = P_{NM}(1 - f_{resM_j}) L_j \frac{M_j k_{INM_j}}{\Delta z_{bot}} \quad (7.21)$$

$$E_{NO_3}(M_j) = (1 - P_{NM})(1 - f_{resM_j}) L_j \frac{M_j k_{INM_j}}{\Delta z_{bot}} \quad (7.22)$$

$$E_{PO_4}(M_j) = (1 - f_{resM_j}) L_j \frac{M_j k_{IPM_j}}{\Delta z_{bot}} \quad (7.23)$$

$$E_{PONL}(M_j) = E_{PONL}^{BW}(M_j) \quad (7.24)$$

$$E_{POPL}(M_j) = E_{POPL}^{BW}(M_j) \quad (7.25)$$

where f_{resM_j} is the fraction of the total loss that is respiration of CO_2 for macroalgal group, j , $E_{POCL}^{BW}(M_j)$, $E_{PONL}^{BW}(M_j)$, $E_{POPL}^{BW}(M_j)$ are the contribution of dead macroalgae to $POCL$, $PONL$ and $POPL$ respectively, created through the process of beach wrack (see below), and the nutrient parameters have been defined previously.

When the hydrodynamic driver is three-dimensional (e.g. ELCOM), a transfer function is adopted that transports macroalgae between grids based on a fixed fraction of the horizontal velocities at the sediment-water interface. The velocities are computed by the hydrodynamics module. For the purposes of the macroalgae model, additional grid points are added surrounding the water, to constitute ‘beach’. When the computed position of macroalgae indicates that the biomass is outside the usual boundaries for water in the model, macroalgae are removed from the water. The material removed constitutes beach wrack (the removal will implicitly include an adjustment for the fact around 10% of the macroalgal biomass is returned to the water column as viable biomass). The beach wrack is incremented over the course of the day until midnight, when it is reset to 5% of its mass at that time. This is done to represent return of dead macroalgae to the water at high tide. The dead macroalgae is then represented in terms of their nutrient content and equivalent POC. Therefore there is a change in nutrient concentration in the layer nearest the shore, which is associated with the entry of nutrients and POC from the beach wrack, modelled

as:

$$E_{POCL}^{BW}(M_j) = \frac{WL_j}{h_{mac}} \quad (7.26)$$

$$E_{PONL}^{BW}(M_j) = \frac{WL_j k_{INM_j}}{h} \quad (7.27)$$

$$E_{POPL}^{BW}(M_j) = \frac{WL_j k_{IPM_j}}{h} \quad (7.28)$$

where $WL = 0.9M_j$, h is the depth of the layer closest to the shore and k_{INM_j} and k_{IPM_j} represent ratios of internal nitrogen and phosphorus in the beach wrack. The beach wrack functions are added to the water over the six hours following midnight to avoid a sudden pulse of nutrients or carbon entering the water.

7.2.3 Grazing: Removal of macroalgae through grazing is solely via crustacean grazers, GZ . For crustaceans the weighted grazing $f(W)$ on macroalgae (since they may also graze on epiphytes associated with seagrasses) is:

$$f(W)_j = \frac{P_{gzj}M_j}{\sum_j^{nmac} [P_{gzj}M_j] + (1 - \sum P_{gzj})f_e SG} \quad (7.29)$$

where P_{gzj} is the preference of crustacean grazers for macroalgal group j , $(1 - \sum P_{gzj})$ is the preference of crustaceans for seagrass epiphytes, f_e is the ratio of carbon of epiphytes to carbon of seagrass, and SG is the seagrass biomass. The overall rate of grazing by crustaceans is regulated according to a Michaelis-Menten function of the form:

$$f_{GZ}(Z) = \frac{\sum_j^{nmac}(M_j) + f_e SG}{K_{GZ} + \sum_j^{nmac}(M_j) + f_e SG} \quad (7.30)$$

where K_{GZ} is the half saturation constant for crustaceans grazing on seagrass and macroalgae ($g C m^{-2}$). Therefore the equation to describe the rate of removal of macroalgae due to grazing by crustaceans is:

$$G_j = GRZ f_{GZ}(Z) f(W)_j f_{GZ}(T) GZ \quad (7.31)$$

where GZ is the crustacean biomass ($g C m^{-2}$), GRZ is the maximum consumption rate ($g C$ consumed (g crustacean C) $^{-1} day^{-1}$) of the grazers, which is regulated by a temperature function $f_{GZ}(T)$, which includes inhibition at high temperatures.

7.3 Seagrass & Macrophytes

CAEDYM includes as a state variable one group of seagrasses or macrophytes. Much of the following introduction and the derivation of algorithms is adapted from Hillman et al. (1995). The main factors influencing the biomass and production of *Halophila ovalis* in the Swan-Canning are light, temperature and salinity. Therefore, for any application where macrophyte abundance is not controlled by nutrient limitation (since the roots have free access to the sediments), this state variable may be considered appropriate.

The biomass of this state variable is represented as $g C m^{-2}$. The seagrass algorithm is based on the study of Hillman et al. (1995), in which laboratory experiments were conducted to relate productivity to changes in light, temperature and salinity. These experiments were based on a constant light source over a 12 hour photoperiod and provided net productivity over a 24 hour period. It is desirable to simulate macrophyte growth over a much smaller time scale so that chemical interactions (specifically denitrification) can be resolved during times when seagrass are net consumers of oxygen (night-time) and net producers of oxygen (day-time). The equation for seagrasses/macrophytes is written as:

$$\frac{\partial SG}{\partial t} = \epsilon_{max} f_{SG}(I) f_{SG}(T) - k_{rSG} \vartheta^{T-20} f_{SG}(S) \quad (7.32)$$

where SG is the seagrass/macrophyte biomass ($g C m^{-2}$), ϵ_{max} is the maximum productivity (day^{-1}), $f_{SG}(I)$ is the Webb et al. (1974) light limitation function, defined as:

$$f_{SG}(I) = 1 - \exp\left(\frac{-I}{I_k}\right) \quad (7.33)$$

where I is the photosynthetically active radiation ($mE m^{-2} s^{-1}$) and I_k is a constant. The function, $f_{SG}(T)$ is a temperature function of the form of 6.9 and solved in a similar manner. The parameter, k_{rSG} is the respiration rate (day^{-1}), and $f_{SG}(S)$ is a salinity, S , dependence of the form:

$$f_{SG}(S) = \frac{(\beta - \alpha)}{S_{opt}^2} S^2 - 2 \frac{(\beta - \alpha)}{S_{opt}} S + \beta \quad (7.34)$$

where S_{opt} is the optimum salinity for maximum growth, $\beta = f(0)$ and $\alpha = f(S_{opt})$. The constants were set so that when the seagrass model was used subject to the same conditions imposed by Hillman et al. (1995), the resulting productivity correlated with that measured by Hillman et al. However, Hillman et al. (1995) used a base respiration of $-0.67 mg dw apex^{-1} day^{-1}$ (for $I = 0$), which was derived via a linear regression on the measured P-I curve. Since the P-I curve is non-linear, it is appropriate to fit a non-linear curve of the Webb et al. (1974) form to approximate production in the absence of light, which gives a base respiration of $-0.93 mg dw apex^{-1} day^{-1}$. The P-I data suggests that the upper limit of production approaches 3.1 as $I \rightarrow \inf$. Also the data of Hillman et al. (1995) exhibit inconsistencies when experiments were conducted with overlapping data (i.e. production was measured as 1.1, 2.1 and 2.4 $dw apex^{-1} day^{-1}$ when $I = 120 mE m^{-2} s^{-1}$, $T = 25^\circ C$ and $S = 35ppt$ in three different experiments, the mean, equal to 1.9, of these was used). A modified P-I curve was generated taking the above into consideration, and the model constants were chosen so as simulated production correlated with production measured by Hillman et al. (1995).

The photoperiod correction is used to allow application of the P-I curve given by Hillman et al. (1995) was arrived at for simulated photoperiods of 12 hours. The depth-integrated mean PAR over the photoperiod is arrived at from the depth of water and the light extinction coefficient.

The value of light reaching the top of the bottom layer is determined as:

$$I(1) = I(2) \exp(-K_d \Delta z) \quad (7.35)$$

where $I(1)$ is the PAR at the top of the bottom layer as a mean for each hour, $I(2)$ is the PAR at the top of the second layer above the bottom as a mean for each hour, Δz is the grid cell depth and K_d is the attenuation coefficient, and is arrived at according to:

$$\begin{aligned} K_d &= K_w \text{ attenuation due to pure water - constant} \\ &+ \sum_i^{nphy} K_{A_i} \text{ specific attenuation due to phytoplankton groups} \\ &+ \sum_b^{ndom} K_{DOC_b} \text{ specific attenuation due to dissolved organic carbon} \\ &+ \sum_b^{npom} K_{POC_b} \text{ specific attenuation due to particulate organic matter} \\ &+ \sum_s^{nsol} K_{SS_s} \text{ specific attenuation due to inorganic particles} \end{aligned} \quad (7.36)$$

The height of the macroalgae layer, h is determined (see Section 7.2 and the light reaching the top of the macroalgal $I(mb)$ is determined as:

$$I(mb) = I(1) \exp[-K_d(\Delta z - h)] \quad (7.37)$$

where $I(1)$ is the light reaching the top of the bottom-most layer, K_d is the light attenuation coefficient determined as given by the formula above, and Δz is the grid thickness of the bottom-most layer.

A new value of K_d is defined for within the macroalgae bed:

$$\begin{aligned} K_d &= K_w (\text{attenuation due to pure water - constant}) \\ &+ \sum_i^{nphy} K_{A_i} \text{ specific attenuation due to phytoplankton groups} \\ &+ \sum_b^{ndom} K_{DOC_b} \text{ specific attenuation due to dissolved organic carbon} \\ &+ \sum_b^{npom} K_{POC_b} \text{ specific attenuation due to particulate organic matter} \\ &+ \sum_s^{nsol} K_{SS_s} \text{ specific attenuation due to inorganic particles} \\ &+ \sum_j^{nmac} K_{M_j} \text{ specific attenuation due to macroalgae} \end{aligned} \quad (7.38)$$

The light available to the seagrasses is then determined (macroalgae are ignored if they are not present). Note that the attenuation is identical to that used for phytoplankton except for the inclusion of macroalgal biomass (as gm^{-2}), with specific attenuation coefficients expressed in mg^{-1} instead of $m^2 g^{-1}$ as for light attenuating components of the water column. Epiphytes are not considered to be very important in colonising *Halophila* and influencing the availability of light (Hillman et al., 1995).

7.4 Macroinvertebrates

7.4.1 Bivalves: The bivalve model includes grazing on phytoplankton and detritus, respiration and predation by fish. This is represented as:

$$\begin{aligned} \frac{\partial BV}{\partial t} = & \left[GBZ f_{BV}(T) BV f_{BV}(S) \frac{\sum_i^{nphy} (A_i Y_{C:Chla}) + \sum_b^{npom} POC_b}{K_{BV} + \sum_i^{nphy} (A_i Y_{C:Chla}) + \sum_b^{npom} POC_b} \right] \\ & - k_{r_{BV}} \vartheta^{T-20} f_{BV}(DO) BV - G_{BV} \end{aligned} \quad (7.39)$$

where BV is the bivalve biomass ($g C m^{-2}$), GBZ is the maximum consumption rate ($g C$ consumed (g bivalve C) $^{-1}$), $f_{BV}(T)$ is a temperature function of the form of 6.9, and $f_{BV}(S)$ is the grazing response to salinity, defined as:

$$\begin{aligned} f_{BV}(S) &= 1.0 : S_{min} \leq S \leq S_{max} \\ f_{BV}(S) &= -\frac{S}{S_{max}^2} + 2\frac{S}{S_{min}} : S < S_{min} \\ f_{BV}(S) &= \frac{-S^2 + 2S_{max}S - 2S_{max}max_s + max_s^2}{(S_{max} - max_s)^2} : S > S_{max} \end{aligned}$$

where max_s is the upper limit of salinity where no grazing occurs. The parameter K_{BV} , is the half-saturation constant for bivalve grazing response to food abundance, and $k_{r_{BV}}$ is the respiration rate constant (day^{-1}) and the respiration losses are mediated by a dissolved oxygen dependence:

$$f_{BV}(DO) = 1 - \beta \frac{K_{DO-BV}}{K_{DO-BV} + DO} \quad (7.40)$$

where K_{DO-BV} regulates the response of respiration losses to DO in the bottom layer.

Predation by the fish, G_{BV} , is modelled as:

$$G_{BV} = \sum_f^{nfish} k_f f_f(F) f(W)_{BV} f_f(T) F_f \quad (7.41)$$

where k_f is the rate of grazing of fish group f ($g C$ consumed (g fish C) $^{-1}$), F_f is the fish concentration for group f ($mg C L^{-1}$), $f_f(F)$ is a Michaelis-Menten function that controls the rate of the fish groups, defined as:

$$f(F_f) = \frac{\sum_i^{nphy} A_i Y_{C:Chla} + \sum_k^{nzoo} Z_k + \sum_b^{npom} POC_b + \sum_f^{nfish} F_f + BV + GZ + PC}{K_{F_f} + \sum_i^{nphy} A_i Y_{C:Chla} + \sum_k^{nzoo} Z_k + \sum_b^{npom} POC_b + \sum_f^{nfish} F_f + BV + GZ + PC} \quad (7.42)$$

where K_F controls the fish grazing, and finally, The function $f(W)_{PC}$ is the weighted grazing function for each fish group on polychaetes and is defined by equation 6.86 with $G = P_{fbv} BV$.

7.4.2 Polychaetes: Polychaete biomass, PC , is expressed as $g C m^{-2}$ as with the other benthic variables. Polychaetes are modelled similar to bivalves, except their food preference is slowly decomposing (refractory) detrital material. The equation therefore takes the form:

$$\frac{\partial PC}{\partial t} = \left[GPZ f_{PC}(T) PC \frac{POCR_{sed}}{K_{PC} + POCR_{sed}} \right] - k_{r_{PC}} \vartheta^{T-20} f_{PC}(S) PC - G_{PC} \quad (7.43)$$

where GPZ is the maximum consumption rate of detritus ($g C$ consumed (g polychaete C) $^{-1}$), $f_{PC}(T)$ is a temperature function of the form of 6.9, K_{PC} is the half-saturation constant for polychaetes grazing on detrital material in the sediments, $k_{r_{PC}}$ is the respiration rate coefficient (day^{-1}), G_{PC} is a loss term due to predation by fish (discussed below), and $f_{PC}(S)$ is a salinity dependence for respiration efficiency, given by:

$$f_{PC}(S) = \frac{\beta - 1}{S_{opt}^2} S^2 + \frac{2(\beta - 1)}{S_{opt}} S + \beta \quad (7.44)$$

where β is the value of $f_{PC}(S)$ when the salinity is zero, and S_{opt} is the salinity at which $f_{PC}(S)$ is 1.0 (i.e. the minimum value of $f_{PC}(S)$). This expression is parabolic, such that it acts to increase the respiration rate as salinities decrease below S_{opt} or as they increase above S_{opt} .

The mortality due to predation by fish, G_{PC} , is described by:

$$G_{PC} = \sum_f^{n_{fsh}} [k_f f_f(F) f(W)_{PC} f_f(T) F_f] \quad (7.45)$$

where k_f is the maximum grazing rate of the fish ($g C$ consumed (g fish C) $^{-1}$), F_f is the fish concentration for group f ($mg C L^{-1}$), $f_f(F)$ is a Michaelis-Menten function that controls the rate of fish grazing, defined as:

$$f(F_f) = \frac{\sum_i^{n_{phy}} A_i Y_{C:Chla} + \sum_k^{n_{zoo}} Z_k + \sum_b^{n_{pom}} POC_b + \sum_f^{n_{fsh}} F_f + BV + GZ + PC}{K_{F_f} + \sum_i^{n_{phy}} A_i Y_{C:Chla} + \sum_k^{n_{zoo}} Z_k + \sum_b^{n_{pom}} POC_b + \sum_f^{n_{fsh}} F_f + BV + GZ + PC} \quad (7.46)$$

where K_{F_f} controls the fish grazing. The function $f(W)_{PC}$ is the weighted grazing function for each fish group on polychaetes and is defined by equation 6.86 with $G = P_{fpc} PC$.

7.4.3 Crustacean Grazers: The biomass of crustacean grazers will be regulated largely by the epiphyte biomass and the macroalgae density. Epiphytes are not at present represented explicitly in the model. However, in the case of the Swan River, for example, most of the epiphyte biomass in the is associated with seagrasses. Hillman et al. (1985) suggested that epiphytes associated with *Halophila ovalis* were relatively unimportant due to the fast growth of the seagrass. More recent evidence indicates that epiphytes are in fact quite abundant on *Halophila* around May, although it is not known if this is a regular annual occurrence. A compromise is currently proposed; epiphytes will not be simulated as a state variable, but the biomass increment of crustacean grazers will be dependent on the biomass of seagrasses, assuming that there is a direct linear dependence between epiphyte and seagrass biomass. The equation for crustacean biomass is therefore:

$$\begin{aligned} \frac{\partial GZ}{\partial t} &= \left[GRZ f_{GZ}(T) GZ \frac{\sum_j^{n_{mac}} M_j + f_e SG}{K_{GZ} \sum_j^{n_{mac}} M_j + f_e SG} \right] \\ &- k_{r_{GZ}} \vartheta^{T-20} f_{GZ}(S) GZ - f_{GZ}(DO) - G_{GZ} \end{aligned} \quad (7.47)$$

where GRZ is the maximum grazing rate ($g C$ consumed (g crustacean C) $^{-1}$), $f_{GZ}(T)$ is a temperature function of the form of 6.9, K_{GZ} is the half-saturation constant for crustaceans grazing on epiphytes and macroalgae, f_e is the

ratio of carbon of epiphytes to carbon of seagrasses/macrophytes, $k_{r_{GZ}}$ is the respiration rate coefficient (day^{-1}), G_{GZ} is a loss term due to predation by fish (discussed below), and $f_{GZ}(S)$ is a salinity dependence for respiration efficiency, given by:

$$f_{GZ}(S) = \frac{\beta - 1}{S_{opt}^2} S^2 + \frac{2(\beta - 1)}{S_{opt}} S + \beta \quad (7.48)$$

where β is the value of $f_{GZ}(S)$ when the salinity is zero, and S_{opt} is the salinity at which $f_{GZ}(S)$ is 1.0 (i.e. the minimum value of $f_{GZ}(S)$). This expression is parabolic, such that it acts to increase the respiration rate as salinities decrease below S_{opt} or as they increase above S_{opt} . The dissolved oxygen function, $f_{GZ}(DO)$ is of the form:

$$f_{GZ}(DO) = 1 - \beta \frac{K_{DO-GZ}}{K_{DO-GZ} + DO} \quad (7.49)$$

where K_{DO-GZ} is a value of dissolved oxygen that regulates the shape of the response curve and β dictates the sensitivity of the response to a depletion in DO.

The mortality due to predation by fish, G_{PC} , is described by:

$$G_{GZ} = \sum_f^{nfsh} [k_f f_f(F) f(W)_{GZ} f_f(T) F_f] \quad (7.50)$$

where k_f is the maximum grazing rate of the fish ($g C$ consumed (g fish C) $^{-1}$), F_f is the fish concentration for group f ($mg C L^{-1}$), $f_f(F)$ is a Michaelis-Menten function that controls the rate of fish grazing, defined as:

$$f(F_f) = \frac{\sum_i^{nphy} A_i Y_{C:Chla} + \sum_k^{nzoo} Z_k + \sum_b^{npom} POC_b + \sum_f^{nfsh} F_f + BV + GZ + PC}{K_{F_f} + \sum_i^{nphy} A_i Y_{C:Chla} + \sum_k^{nzoo} Z_k + \sum_b^{npom} POC_b + \sum_f^{nfsh} F_f + BV + GZ + PC} \quad (7.51)$$

where K_{F_f} controls the fish grazing. The function $f(W)_{GZ}$ is the weighted grazing function for each fish group on polychaetes and is defined by equation 6.86 with $G = P_{fgz} GZ$.

7.5 Clams and Mussels

The clam model includes grazing on phytoplankton and detritus, respiration and predation by fish. This is represented as:

$$\begin{aligned} \frac{\partial CLM_c}{\partial t} &= (1 - k_{e_c}) \left[\mu_{CLM_c} f_c(T) f_c(S) \frac{\sum_i^{nphy} (A_i Y_{C:Chla}) + \sum_b^{npom} POC_b}{K_{CLM_c} + \sum_i^{nphy} (A_i Y_{C:Chla}) + \sum_b^{npom} POC_b} \right] CLM_c \\ &- (k_{r_c} + k_{m_c}) \vartheta^{T-20} f_c(DO) CLM_c - G_{CLM_c} \end{aligned} \quad (7.52)$$

where CLM_c is the clam biomass ($g C m^{-2}$) for clam group c , μ_{CLM_c} is the maximum consumption rate ($g C$ consumed (g clam C) $^{-1}$), $f_c(T)$ is a temperature function regulating consumption, and $f_c(S)$ is the grazing response to salinity for group c , defined as:

$$f_c(S) = \begin{cases} 0.0 & S \leq S_{MIN} \\ \frac{-(S - S_{MIN})^2 / S_{\alpha_c}^2 + 2(S - S_{MIN}) / S_{\alpha_c}}{-(S_{\alpha_c} - S_{MIN})^2 / S_{\alpha_c}^2 + 2(S_{\alpha_c} - S_{MIN}) / S_{\alpha_c}} & S_{MIN} < S < S_{\alpha_c} \\ 1.0 & S_{\alpha_c} \leq S \leq S_{\beta_c} \\ \frac{-S^2 + 2S_{\beta_c} S - 2S_{\beta_c} S_{MAX} + S_{MAX}^2}{(S_{\beta_c} - S_{MAX})^2} & S_{\beta_c} < S < S_{MAX} \\ 0.0 & S \geq S_{MAX} \end{cases} \quad (7.53)$$

where S_α is the minimum salinity within the optimal range, S_β is the maximum salinity within the optimal range and S_{MAX} is the maximum tolerable salinity, beyond which, the clam shells are considered to be completely closed and food intake does not occur. Clams feed within the bottom layer only, on all simulated algae, A , and detrital, POC , groups ($nphy$ and $npom$ indicate the number of simulated phytoplankton and detrital groups respectively). Since they are filter feeders, no preference is given to particular food groups and food is ingested indiscriminately. Algal and detrital uptake is in carbon units so $Y_{C:Chla}$ is used to convert algal chlorophyll to carbon, and the uptake is modelled using a Michaelis-Menten function with K_{CLM_c} defined as the half-saturation constant for clam grazing response to food abundance ($g C m^{-3}$) for group c . Of the food that is ingested, a prescribed fraction, k_e , is lost directly as faecal pellets via egestion and returned to the detrital pool within the benthos.

The loss terms in 7.52 include respiration, k_r , and natural mortality, k_m . The loss rates are mediated by a temperature dependence and are enhanced under poor oxygen conditions according to:

$$f_c(DO) = 1 + \beta_c \frac{K_{DO_c}}{K_{DO_c} + DO} \quad (7.54)$$

where DO is the dissolved oxygen concentration ($g O_2 m^{-3}$), K_{DO} regulates the effects of anoxia and β is the maximum possible respiration/mortality enhancement under complete anoxia. If required, CAEDYM also allows for clam predation by fish, G_{CLM} , as an additional loss mechanism and this is modelled as:

$$G_{CLM_c} = \sum_f^{nfs} k_f f_f(F) f(W)_{CLM_c} f_f(T) F_f; \quad (7.55)$$

refer to the fish section for more detail.

So that the average clam size/length can be determined, CAEDYM additionally simulates a state variable for each group that models the evolution of clam numbers, $NCLM$, simply modeled as:

$$\frac{\partial NCLM_c}{\partial t} = - (k_{m_c} \vartheta^{T-20} f_c(DO) + G_{CLM_c}) NCLM_c \quad (7.56)$$

Note that clam numbers only change due to mortality; respiratory losses do not reduce clam numbers, only clam biomass. Currently the effects of spawning and reproduction as increases to the number of clams is not included.

Metals

8.1 Iron

A simple formulation for iron is used here. The model is to be replaced in CAEDYM v3 where a full geochemistry sub-model has been linked in. The effect of oxidation of metals is not included in the oxygen budget at present as changes due to this process are generally 2-3 orders of magnitude less than those commonly observed with changes oxygen due to mineralisation of organic matter or photosynthesis. The equation for the change in Fe^{2+} is given as:

$$\frac{\partial Fe^{2+}}{\partial t} = k_{FeR} \vartheta_{FeR}^{T-20} \frac{K_{FeR}}{K_{FeR} + DO} (TFe - Fe^{2+}) - k_{FeO} \vartheta_{FeO}^{T-20} \frac{DO}{K_{FeO} + DO} (Fe^{2+}) + f_{Fe^{2+}}^{DSF} \quad (8.1)$$

where Fe^{2+} is iron in dissolved form ($mg L^{-1}$), TFe is total iron (including Fe^{2+} and Fe^{3+}), k_{FeR} is the maximum reduction rate of Fe^{3+} at $20^\circ C$ (day^{-1}), k_{FeO} is the maximum oxidation rate at $20^\circ C$ (day^{-1}), ϑ_{FeR} and ϑ_{FeO} are temperature multipliers for the oxidation and reduction reactions and K_{FeR} and K_{FeO} regulate transitions between Fe^{2+} and Fe^{3+} according to the availability of oxygen.

Release of iron from the sediments, $f_{Fe^{2+}}^{DSF}$ is in the dissolved form and is modelled within the layer/cell adjacent to the sediment only as with the nutrient fluxes:

$$f_{Fe^{2+}}^{DSF} = S_{Fe} \left[\frac{K_{DO-Fe}}{K_{DO-Fe} + DO} + \frac{|pH - 7|}{K_{pH-Fe} + |pH - 7|} \right] \frac{1}{dz_{bot}} \quad (8.2)$$

where S_{Fe} is the release rate ($g m^{-2} day^{-1}$) and K_{DO-Fe} and K_{pH-Fe} regulate the release rate according to the dissolved oxygen and pH in the layer above the sediments (which has depth dz_{bot}).

The total iron equation includes fluxes for resuspension and sedimentation of the particulate iron, and the sediment flux from the dissolved component:

$$\frac{\partial TFe}{\partial t} = f_{Fe^{3+}}^{RES} + f_{Fe^{2+}}^{DSF} + \frac{v_{s_{Fe}}}{\Delta z} (TFe - Fe^{2+}) \quad (8.3)$$

where $v_{s_{Fe}}$ is the settling velocity for particulate iron, which adjusted to account for changes in the density and viscosity following similar equations as outlined above for other particulate components within CAEDYM. The resuspension of iron by currents and wave action is also modelled as with the other particulate variables:

$$f_{Fe^{3+}}^{RES} = \alpha_{Fe} \left[\frac{\tau - \tau_{c_{Fe}}}{\tau_{ref}} \right] \left[\frac{(TFe - Fe^{2+})_{sed}}{K_{Fe} + (TFe - Fe^{2+})_{sed}} \right] \frac{1}{dz_{bot}} \quad (8.4)$$

where α_{Fe} is the resuspension rate constant (discussed in more detail in Section 10.2), which has units of $g m^{-2} s^{-1}$, $\tau_{c_{Fe}}$ is the critical shear stress for particulate iron ($N m^{-2}$), τ_{ref} is a reference shear stress and K_{Fe} controls the rate of resuspension based on the amount of sediment mass available.

8.2 Manganese

Manganese is modelled in a similar fashion to iron. Again, the model is intended to be further developed and increased process representation added with successive applications. The equation for the change in Mn^{2+} is given as:

$$\frac{\partial Mn^{2+}}{\partial t} = k_{MnR} \vartheta_{MnR}^{T-20} \frac{K_{MnR}}{K_{MnR} + DO} (TMn - Mn^{2+}) - k_{MnO} \vartheta_{MnO}^{T-20} \frac{DO}{K_{MnO} + DO} (Mn^{2+}) + f_{Mn^{2+}}^{DSF} \quad (8.5)$$

where Mn^{2+} is manganese in dissolved form ($mg L^{-1}$), TMn is total manganese (including Mn^{2+} and Mn^{3+}), k_{MnR} is the maximum reduction rate of Mn^{3+} at $20^\circ C$ (day^{-1}), k_{MnO} is the maximum oxidation rate at $20^\circ C$ (day^{-1}), ϑ_{MnR} and ϑ_{MnO} are temperature multipliers for the oxidation and reduction reactions and K_{MnR} and K_{MnO} regulate transitions between Mn^{2+} and Mn^{3+} according to the availability of oxygen.

Release of manganese from the sediments, $f_{Mn^{2+}}^{DSF}$ is in the dissolved form and is modelled within the layer/cell adjacent to the sediment only as with the nutrient fluxes:

$$f_{Mn^{2+}}^{DSF} = S_{Mn} \left[\frac{K_{DO-Mn}}{K_{DO-Mn} + DO} + \frac{|pH - 7|}{K_{pH-Mn} + |pH - 7|} \right] \frac{1}{dz_{bot}} \quad (8.6)$$

where S_{Mn} is the release rate ($g m^{-2} day^{-1}$) and K_{DO-Mn} and K_{pH-Mn} regulate the release rate according to the dissolved oxygen and pH in the layer above the sediments (which has depth dz_{bot}).

The total manganese equation includes fluxes for resuspension and sedimentation of the particulate manganese, and the sediment flux from the dissolved component:

$$\frac{\partial TMn}{\partial t} = f_{Mn^{3+}}^{RES} + f_{Mn^{2+}}^{DSF} + \frac{v_{sMn}}{\Delta z} (TMn - Mn^{2+}) \quad (8.7)$$

where v_{sMn} is the settling velocity for particulate manganese, which is adjusted to account for changes in the density and viscosity following similar equations as outlined above for other particulate components within CAEDYM. The resuspension of sediment manganese by currents and wave action is also modelled as with the other particulate variables:

$$f_{Mn^{3+}}^{RES} = \alpha_{Mn} \left[\frac{\tau - \tau_{cMn}}{\tau_{ref}} \right] \left[\frac{(TMn - Mn^{2+})_{sed}}{K_{Mn} + (TMn - Mn^{2+})_{sed}} \right] \frac{1}{dz_{bot}} \quad (8.8)$$

where α_{Mn} is the resuspension rate constant (discussed in more detail in Section 10.2), which has units of $g m^{-2} s^{-1}$, τ_{cMn} is the critical shear stress for particulate manganese ($N m^{-2}$), τ_{ref} is a reference shear stress and K_{Mn} controls the rate of resuspension based on the amount of sediment mass available.

8.3 Aluminium

Aluminium is modelled in a similar fashion to the other metals, but instead of representing oxidation states, the particulate and dissolved components are used to represent precipitate and dissolved phases. Again, the model

is intended to be further developed and increased process representation added with successive applications. The equation for the change in Al^{3+} is given as:

$$\frac{\partial Al^{3+}}{\partial t} = k_{AlR} \vartheta_{AlR}^{T-20} \frac{K_{AlR}}{K_{AlR} + DO} (TAI - Al^{3+}) - k_{AlO} \vartheta_{AlO}^{T-20} \frac{DO}{K_{AlO} + DO} (Al^{3+}) + f_{Al^{3+}}^{DSF} \quad (8.9)$$

where Al^{3+} is aluminium in dissolved form ($mg L^{-1}$), TAI is total aluminium, k_{AlR} is the maximum dissolution rate of Al^{3+} at $20^\circ C$ (day^{-1}), k_{AlO} is the maximum precipitation rate at $20^\circ C$ (day^{-1}), ϑ_{AlR} and ϑ_{AlO} are temperature multipliers for the conversion processes and K_{AlR} and K_{AlO} regulate transitions between dissolved and precipitate components according to the availability of oxygen (as a proxy for pH).

Release of aluminium from the sediments, $f_{Al^{3+}}^{DSF}$ is in the dissolved form and is modelled within the layer/cell adjacent to the sediment only as with the nutrient fluxes:

$$f_{Al^{3+}}^{DSF} = S_{Al} \left[\frac{K_{DO-Al}}{K_{DO-Al} + DO} + \frac{|pH - 7|}{K_{pH-Al} + |pH - 7|} \right] \frac{1}{dz_{bot}} \quad (8.10)$$

where S_{Al} is the release rate ($g m^{-2} day^{-1}$) and K_{DO-Al} and K_{pH-Al} regulate the release rate according to the dissolved oxygen and pH in the layer above the sediments (which has depth dz_{bot}).

The total aluminium equation includes fluxes for resuspension and sedimentation of the particulate aluminium, and the sediment flux from the dissolved component:

$$\frac{\partial TAI}{\partial t} = f_{Al}^{RES} + f_{Al^{3+}}^{DSF} + \frac{v_{sAl}}{\Delta z} (TAI - Al^{3+}) \quad (8.11)$$

where v_{sAl} is the settling velocity for particulate aluminium, which is adjusted to account for changes in the density and viscosity following similar equations as outlined above for other particulate components within CAEDYM. The resuspension of sediment aluminium by currents and wave action is also modelled as for the other particulate variables:

$$f_{Al}^{RES} = \alpha_{Al} \left[\frac{\tau - \tau_{cAl}}{\tau_{ref}} \right] \left[\frac{(TAI - Al^{3+})_{sed}}{K_{Al} + (TAI - Al^{3+})_{sed}} \right] \frac{1}{dz_{bot}} \quad (8.12)$$

where α_{Al} is the resuspension rate constant (discussed in more detail in Section 10.2), which has units of $g m^{-2} s^{-1}$, τ_{cAl} is the critical shear stress for particulate aluminium ($N m^{-2}$), τ_{ref} is a reference shear stress and K_{Al} controls the rate of resuspension based on the amount of sediment mass available.

Pathogens

9.1 Cryptosporidium

The *Cryptosporidium* model developed within CAEDYM is discussed in some detail in Hipsey et al. (2004), and a comprehensive review of pathogen dynamics in lakes and reservoirs is given by Brookes et al. (2003). The model allows for oocyst settling and resuspension, and inactivation via natural mortality (temperature dependent) and through exposure to different bandwidths of ultra-violet (UV) light (Figure 9.1):

$$\frac{\partial C}{\partial t} = \left[-f_C^{INA}(UV) - f_C^{INA}(T) + \frac{v_{sC}}{\Delta z} \right] + f_C^{RES} \quad (9.1)$$

where C is the *Cryptosporidium* oocyst concentration (*oocysts* $(10L)^{-1}$), $f_C^{INA}(UV)$ is a function that models the inactivation through UV exposure, $f_C^{INA}(T)$ is a function that models inactivation through exposure to non-optimum temperature, v_{sC} is the oocyst settling velocity ($m s^{-1}$) and f_C^{RES} is the usual resuspension function, defined as:

$$f_C^{RES} = \alpha_C \left[\frac{\tau - \tau_{cC}}{\tau_{ref}} \right] \left[\frac{C_{SED}}{K_{TC} + C_{SED}} \right]; \quad (9.2)$$

where α_C is the resuspension rate constant ($g m^{-2} s^{-1}$), τ_{cC} is the critical shear stress ($N m^{-2}$), τ_{ref} is a reference shear stress and K_{TC} controls the rate of resuspension based on the amount of sediment mass available.

In the code there is capacity to model inactivation by light for upto three different bandwidths, but in the CAEDYM v2.2 public executables only one bandwidth is enabled. In this version, the inactivation functions are modelled as:

$$f_C^{INA}(UV) = e^{-k_{UV} I_{UV} t} \quad (9.3)$$

$$f_C^{INA}(T) = e^{-k_T t} \quad (9.4)$$

where k_{UV} is the sensitivity parameter of the oocysts to the particular bandwidth of UV light, I_{UV} is the intensity of the incoming UV ($W m^{-2}$), t is time, and k_T is defined empirically as:

$$k_T = 10^{-2.68} 10^{0.058T} \quad (9.5)$$

where T is temperature in degrees Celcius. The pathogen module within CAEDYM allows for 3 different pathogen classes, each of which have state variables for the viable and inactivated oocysts. This way, oocyst distribution can be compared with fate processes. If the user enables more than two groups, the oocysts will dynamically aggregate onto the suspended particles, SSOL1 and SSOL2. The attached group will then settle at the rate of the suspended particles. For more information refer to Hipsey et al. (2004).

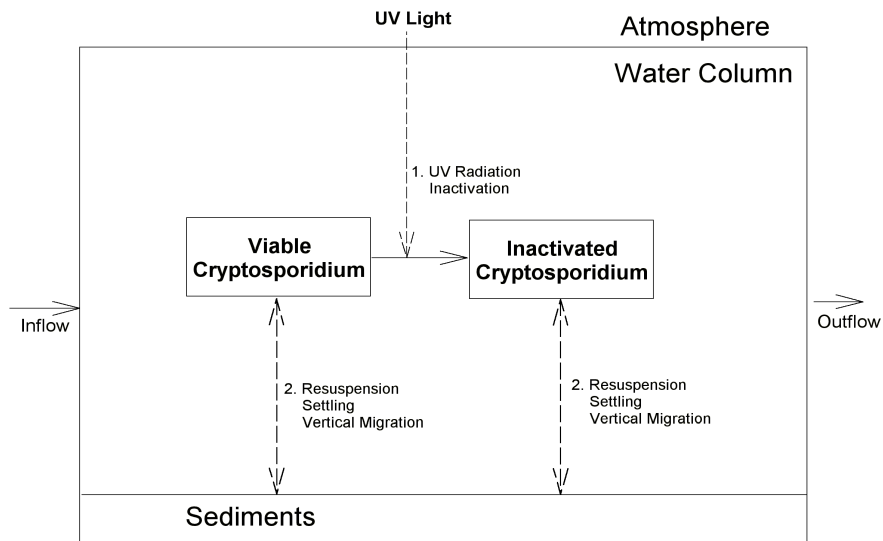


Figure 9.1 Schematic of *Cryptosporidium* dynamics within CAEDYM.

9.2 Faecal Bacteria

In the CAEDYM v2.2 code, facility exists to switch the pathogen model from Crypto to coliform (or other) bacteria. The model is basically similar to that described above, however, the bacteria are also sensitive to visible light, and have a mortality temperature function of the form of f^{T^2} . For this release however, users must have access to the source code and compile in specific parameter values. Future releases will expand the usability of this model.

Sediment

10.1 Sediment Composition

CAEDYM v2 differs significantly from previous versions, as now all simulated variables have a sediment component that is fully conserved. The sediment is considered to be a matrix of particulate elements, some of which are captured within CAEDYM and some of which are not. Therefore, CAEDYM requires the user to supply an initial value for the fraction of sediment mass that is organic in nature, f_{org} , and the porosity, ϕ_{sed} . The user is then required to provide values for the particulate sediment components as fractions of the total sediment composition (via the initialisation file). This way CAEDYM can construct a sediment profile and estimate a density that correctly accounts for the various constituents:

$$\begin{aligned} \rho_{sed} = & (1 - \phi_{sed}) \left\{ f_{org} \left(\rho_{POML} \frac{POML}{POML + POMR} + \rho_{POMR} \frac{POMR}{POML + POMR} \right) \right. \\ & \left. + (1 - f_{org}) \left(\rho_{SS1} \frac{SS1}{SS1 + SS2} + \rho_{SS2} \frac{SS2}{SS1 + SS2} \right) \right\} \end{aligned} \quad (10.1)$$

The density of the particulate species (e.g. $POCL$, $POPL$, $PONL$, $SSOL1$, $SSOL2$ etc) is then equal to the user supplied initialisation fraction, γ , multiplied by ρ_{sed} :

$$\rho_{sed_{POCL}} = \gamma_{POCL} \rho_{sed} \quad (10.2)$$

$$\rho_{sed_{POCR}} = \gamma_{POCR} \rho_{sed} \quad (10.3)$$

$$\rho_{sed_{POPL}} = \gamma_{POPL} \rho_{sed} \quad (10.4)$$

$$\rho_{sed_{POPR}} = \gamma_{POPR} \rho_{sed} \quad (10.5)$$

$$\rho_{sed_{PONL}} = \gamma_{PONL} \rho_{sed} \quad (10.6)$$

$$\rho_{sed_{PONR}} = \gamma_{PONR} \rho_{sed} \quad (10.7)$$

$$\rho_{sed_{SSOL1}} = \gamma_{SSOL1} \rho_{sed} \quad (10.8)$$

$$\rho_{sed_{SSOL2}} = \gamma_{SSOL2} \rho_{sed} \quad (10.9)$$

$$\rho_{sed_{Fe}} = \gamma_{Fe} \rho_{sed} \quad (10.10)$$

$$\rho_{sed_{Mn}} = \gamma_{Mn} \rho_{sed} \quad (10.11)$$

$$\rho_{sed_{Al}} = \gamma_{Al} \rho_{sed} \quad (10.12)$$

10.2 Resuspension

10.2.1 Master Resuspension Rate: It is unrealistic to expect users to have resuspension rates for the various classes of particulate species in the sediment (e.g. POM , $SSOL$ etc.). Therefore, CAEDYM only requires a ‘master’ resuspension rate, α , that applies to the overall sediment resuspension:

$$f_{sed}^{RES} = \alpha \frac{\tau - \tau_c}{\tau_{ref}} \frac{\rho_{sed} A}{K_T + \rho_{sed} A} \quad (10.13)$$

where A is area, K_T limits resuspension according to sediment abundance. CAEDYM then proportions the master resuspension rate into its components (excluding phytoplankton and pathogens) according to the compositions discussed above in Section 10.1:

$$\alpha_{POML} = \gamma_{POML} \alpha \quad (10.14)$$

$$\alpha_{POMR} = \gamma_{POMR} \alpha \quad (10.15)$$

$$\alpha_{SSOL1} = \gamma_{SSOL1} \alpha \quad (10.16)$$

$$\alpha_{SSOL2} = \gamma_{SSOL2} \alpha \quad (10.17)$$

$$\alpha_{Fe} = \gamma_{Fe} \alpha \quad (10.18)$$

$$\alpha_{Mn} = \gamma_{Mn} \alpha \quad (10.19)$$

$$\alpha_{Al} = \gamma_{Al} \alpha \quad (10.20)$$

where γ is defined as the mass of the species divided by the total sediment mass for that computational unit (i.e. the fraction of the sediment that is that species). Similarly the half-saturation constant K_T must also be proportioned:

$$K_{POML} = \gamma_{POML} K_T \quad (10.21)$$

$$K_{POMR} = \gamma_{POMR} K_T \quad (10.22)$$

$$K_{SSOL1} = \gamma_{SSOL1} K_T \quad (10.23)$$

$$K_{SSOL2} = \gamma_{SSOL2} K_T \quad (10.24)$$

$$K_{Fe} = \gamma_{Fe} K_T \quad (10.25)$$

$$K_{Mn} = \gamma_{Mn} K_T \quad (10.26)$$

$$K_{Al} = \gamma_{Al} K_T. \quad (10.27)$$

Note that the critical shear stresses are still configurable for each species via the parameters file. The user however, is only required to supply the master resuspension rate, α and a master K_T .

10.2.2 Bottom Shear Stresses: The bed shear stress due to currents and waves is related to the shear velocity, as described by the familiar:

$$\tau = \rho_w u_*^2 \quad (10.28)$$

where τ is the shear stress ($N m^{-2}$) and u_* is the shear velocity in the bottom waters. If we disaggregate the shear velocity into the component caused by steady currents u_{*C} and that caused by wave-induced oscillatory currents u_{*W} , then Beach and Sternberg (1992) defines:

$$\tau = \rho_w (u_{*W}^2 + u_{*C}^2). \quad (10.29)$$

Shear stress for unidirectional steady currents: The shear velocity of a steady current is calculated using the von-Karman-Prandtl "law of the wall" :

$$u_{*c} = \sqrt{\frac{f_c \bar{U}^2}{8}} \quad (10.30)$$

where \bar{U} is the mean current velocity and f_c is a friction factor defined according to:

$$f_c = \frac{0.24}{\left[\log \left(\frac{12h}{k_s} \right) \right]^2} \quad (10.31)$$

where h is the mean water depth, k_s is the bed roughness, given under a flat bed condition as $k_s = 2.5D$ where D is length scale associated with the sediment particles (Engelund and Hansen, 1972).

Shear stress due to oscillatory wave currents: Wind induces a shear on the water surface creating oscillatory wave currents that propagate downward and contribute to the shear stress experienced at the bed. This stress can be estimated by wave-forecasting equations, which are dependant on wind speed, fetch and water depth. The shear velocity created by oscillatory wave currents is estimated from:

$$u_{*w} = \sqrt{0.5 f_w U_{orb}^2} \quad (10.32)$$

where U_{orb} is the maximum orbital velocity (as described below), and f_w is the wave friction factor, defined as (Swart, 1974):

$$f_w = \exp \left[5.213 \left(\frac{k_s}{a} \right)^{0.194} - 5.977 \right] \quad (10.33)$$

with a given as the maximum bottom amplitude, calculated from linear wave theory:

$$a = \frac{H}{2 \sinh \left(\frac{2\pi h}{L} \right)} \quad (10.34)$$

where L is the wave length and H is the wave height. The wave period T is then calculated from

$$T = 1.2 \, 2\pi \frac{U}{g} \tanh(\xi) \tanh \left(\frac{0.0379 \left(\frac{gF}{U^2} \right)^{0.333}}{\tanh(\xi)} \right) \quad (10.35)$$

with:

$$\xi = 0.833 \left(\frac{gh}{U^2} \right)^{0.375} \quad (10.36)$$

where U is the wind velocity 10 m above the water surface, F is the fetch and g is acceleration due to gravity. The wave height is estimated as:

$$H = 0.283 \frac{U^2}{g} \tanh(\zeta) \tanh \left(\frac{0.00565 \left(\frac{gh}{U^2} \right)^{0.5}}{\tanh(\zeta)} \right) \quad (10.37)$$

with:

$$\zeta = 0.53 \left(\frac{gh}{U^2} \right)^{0.75} \quad (10.38)$$

The wave length can be assumed as:

$$L \approx L_0 \sqrt{\tanh \left(\frac{2\pi h}{L_0} \right)} \quad (10.39)$$

and

$$L_0 = \frac{gT^2}{2\pi} . \quad (10.40)$$

The wind-driven surface waves lead to an orbital movement that is translated to the wave bottom or the wave base. The maximum bottom boundary velocity U_{orb} is estimated according to:

$$U_{orb} = \frac{\pi H_s}{T \sinh \left(\frac{2\pi H}{L} \right)} . \quad (10.41)$$

CAEDYM Publications

Table 11.1 briefly summarizes articles where CAEDYM has been presented or used within the literature. If your application/article is not listed here and you would like it to be, please post a message on the online CAEDYM forum: http://www.cwr.uwa.edu.au/services/model_forum/ - Many other un-published applications on a range of water bodies are discussed online.

Table 11.1 Summary of CAEDYM applications published within the literature.

Reference	Focus	Location	Version
Hamilton and Schladow (1997) & Schladow and Hamilton (1997)	Nutrient Cycling, Algal Dynamics	Misc	DYRESM-WQ
Robson and Hamilton (2002) & Robson and Hamilton (2003) & Robson and Hamilton (2004)	Algal Succession, Bloom Dynamics	Swan River Estuary, Australia	v1.4
Chan et al. (2002) & Chan and Hamilton (2001)	Algal Succession, Bloom Dynamics	Swan River Estuary, Australia	v1.4
Antenucci et al. (2003)	Eutrophication Amelioration	San Roque Reservoir, Argentina	v1.4
Romero and Imberger (2003)	Nutrient Cycles, Algal Dynamics	Lake Burragorang, Australia	v1.4
Romero et al. (2003)	Nutrient Cycles, Algal Dynamics	Lake Burragorang, Australia	v1.4
Hillmer and Imberger (2005)	Nutrient Dynamics and Patchiness	Perth Coastal Waters, Australia	v1.4
Gal et al. (2002)	Nutrient Cycles, Algal Dynamics	Lake Kinneret, Israel	v2.0
Bruce et al. (2005)	Zooplankton & Phytoplankton Dynamics	Lake Kinneret, Israel	v2.0
Hipsey et al. (2004)	Pathogen (<i>Cryptosporidium</i>) Dynamics	Myponga Reservoir, Australia	v2.1
Spillman et al. (2005)	Nutrient Budgets, Algal Dynamics	Northern Adriatic Sea, Italy	v2.1

Notation

Table 12.1 variable notation used throughout the CAEDYM v2.2 Science Manual.

Table 12.1: Summary of CAEDYM variable notation.

Variable	Description	Units
<i>A</i>	Phytoplankton C biomass concentration	<i>mg C L⁻¹</i>
<i>AIN</i>	Phytoplankton internal nitrogen concentration	<i>mg N L⁻¹</i>
<i>AIP</i>	Phytoplankton internal phosphorus concentration	<i>mg P L⁻¹</i>
<i>a</i>	Phytoplankton group index	-
<i>N_A</i>	Number of phytoplankton groups being simulated	-
<i>Z</i>	Zooplankton C biomass concentration	<i>mg C L⁻¹</i>
<i>ZIN</i>	Zooplankton internal nitrogen concentration	<i>mg N L⁻¹</i>
<i>ZIP</i>	Zooplankton internal phosphorus concentration	<i>mg P L⁻¹</i>
<i>z</i>	Zooplankton group index	-
<i>N_Z</i>	Number of zooplankton groups being simulated	-
<i>F</i>	Fish C biomass concentration	<i>mg C L⁻¹</i>
<i>FIN</i>	Fish internal nitrogen concentration	<i>mg N L⁻¹</i>
<i>FIP</i>	Fish internal phosphorus concentration	<i>mg P L⁻¹</i>
<i>f</i>	Fish group index	-
<i>N_F</i>	Number of fish groups being simulated	-
<i>B</i>	Bacterial C biomass concentration	<i>mg C L⁻¹</i>
<i>BIN</i>	Bacterial internal nitrogen concentration	<i>mg N L⁻¹</i>
<i>BIP</i>	Bacterial internal phosphorus concentration	<i>mg P L⁻¹</i>
<i>M</i>	Macroalgal C biomass concentration	<i>mg C m⁻²</i>
<i>MIN</i>	Macroalgal internal nitrogen concentration	<i>mg N m⁻²</i>
<i>MIP</i>	Macroalgal internal phosphorus concentration	<i>mg P m⁻²</i>
<i>m</i>	Macroalgae group index	-
<i>N_M</i>	Number of macroalgae groups being simulated	-
<i>BV</i>	Bivalve C biomass concentration	<i>mg C m⁻²</i>
<i>PC</i>	Polychaete C biomass concentration	<i>mg C m⁻²</i>
<i>GZ</i>	Crustacean Grazer C biomass concentration	<i>mg C m⁻²</i>
<i>SG</i>	Seagrass/Macrophyte C biomass concentration	<i>mg C m⁻²</i>
<i>N_D</i>	Number of organic matter groups being simulated	-
<i>d</i>	Detrital organic matter group index	-
<i>DOCL</i>	Dissolved organic carbon concentration (labile)	<i>mg C L⁻¹</i>
<i>POCL</i>	Detrital particulate organic carbon concentration (labile)	<i>mg C L⁻¹</i>
<i>DOCR</i>	Dissolved organic carbon concentration (refractory)	<i>mg C L⁻¹</i>
<i>POCR</i>	Detrital particulate organic carbon concentration (refractory)	<i>mg C L⁻¹</i>
<i>DIC</i>	Dissolved inorganic carbon concentration	<i>mg C L⁻¹</i>
<i>CO₂</i>	Carbon dioxide concentration	<i>mg C L⁻¹</i>
<i>pCO₂</i>	Partial pressure of carbon dioxide	<i>atm</i>
<i>pH</i>	Measure of acidity based on the hydrogen ion concentration, [<i>H⁺</i>]	-
<i>TA</i>	Total alkalinity	<i>mg CaCO₃ L⁻¹</i>
<i>TN</i>	Total nitrogen concentration	<i>mg N L⁻¹</i>
<i>PONL</i>	Detrital particulate organic nitrogen concentration (labile)	<i>mg N L⁻¹</i>
<i>DONL</i>	Dissolved organic nitrogen concentration (labile)	<i>mg N L⁻¹</i>
<i>PONR</i>	Detrital particulate organic nitrogen concentration (refractory)	<i>mg N L⁻¹</i>
<i>DONR</i>	Dissolved organic nitrogen concentration (refractory)	<i>mg N L⁻¹</i>

Continued on Next Page...

Table 12.1 – Continued

Variable	Description	Units
PIN	Particulate inorganic nitrogen concentration	$mg\ N\ L^{-1}$
NH_4	Ammonium concentration	$mg\ N\ L^{-1}$
NO_3	Nitrate concentration	$mg\ N\ L^{-1}$
TP	Total phosphorus concentration	$mg\ P\ L^{-1}$
$POPL$	Detrital particulate organic phosphorus concentration (labile)	$mg\ P\ L^{-1}$
$DOPL$	Dissolved organic phosphorus concentration (labile)	$mg\ P\ L^{-1}$
$POPR$	Detrital particulate organic phosphorus concentration (refractory)	$mg\ P\ L^{-1}$
$DOPR$	Dissolved organic phosphorus concentration (refractory)	$mg\ P\ L^{-1}$
PIP	Particulate inorganic phosphorus	$mg\ P\ L^{-1}$
FRP	Filterable reactive phosphorus	$mg\ P\ L^{-1}$
DO	Dissolved oxygen concentration	$mg\ O\ L^{-1}$
SS	Suspended sediment concentration	$mg\ L^{-1}$
N_S	Number of suspended solid groups being simulated	-
s	Suspended solid group index	-
I_{PAR}, I	Light (PAR) intensity	$\mu E\ m^{-2}$
I_{UV}	Ultra-violet light intensity	$W\ m^{-2}$
T	Temperature	$^{\circ}C$
S	Salinity	psu
Δt	Computational time step day	s
Δz	Vertical thickness of computational cell	m
Δ_{bot}	Vertical thickness of computational cell overlying sediment	m
Δ_{surf}	Vertical thickness of computational cell adjacent to water-atmosphere interface	m

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