

ICM User Guide

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Overview

This user guide provides an introduction to the ICM module coupled in SCHISM model framework. ICM is a water quality model composed of 21 variables including zooplankton, phytoplankton, organic carbon, nitrogen, phosphorus, silica, chemical oxygen demand and dissolved oxygen. It has a long history of application in Chesapeake Bay, US East Coast to simulate the ecosystem in coastal regions and the Bay. The validation of ICM was benefited from the abundant water quality measurements of all kinds of water quality parameters provided from the Bay Program. The coupling of ICM into SCHISM was first done by Yi-Cheng Teng in Virginia Institute of Marine Science. Later on, the development of ICM model was managed by Zhengui Wang from the same institute, particularly the reorganization of the model and an addition of pH module. Apart from the kinetics in the water column, a dynamic sediment flux model of 27 variables is included in ICM, which received particulate organic matter from water column and feedback dissolved inorganic nutrients and sediment oxygen demand. At present, Nicole Cai is introducing a SAV module into the ICM.

1 Workflow for ICM

Figure 1 shows the workflow chart for running SCHISM+ICM model. Usually, a simple grid is encouraged to run the model for the first step. This is because ICM has more than 20 variables and the running time is about 3-4 times of hydrodynamics'. Even though the grid maybe coarse, the result is usually comparable to the one of fine grid model with a much higher running speed. One reason is that most of water quality processes are not very sensitive to high resolution as long as the general transport is correct. If the result is not satisfactory, several measures could be taken into consideration:

- 1) check the grid, redo the grid as necessary
- 2) check the input files. Focus should be put on initial condition, boundary condition and nutrient loading.
- 3) Tuning model parameters.

More information about model setup will be discussed in the sections about ICM input file and model parameters. After the coarse grid ICM model is well calibrated, one can apply the same setup to fine grid which will take much more computation time. In addition, the initial condition of fine grid model can be interpolated from the hotstart.nc (or hotstart.in) of coarse grid.

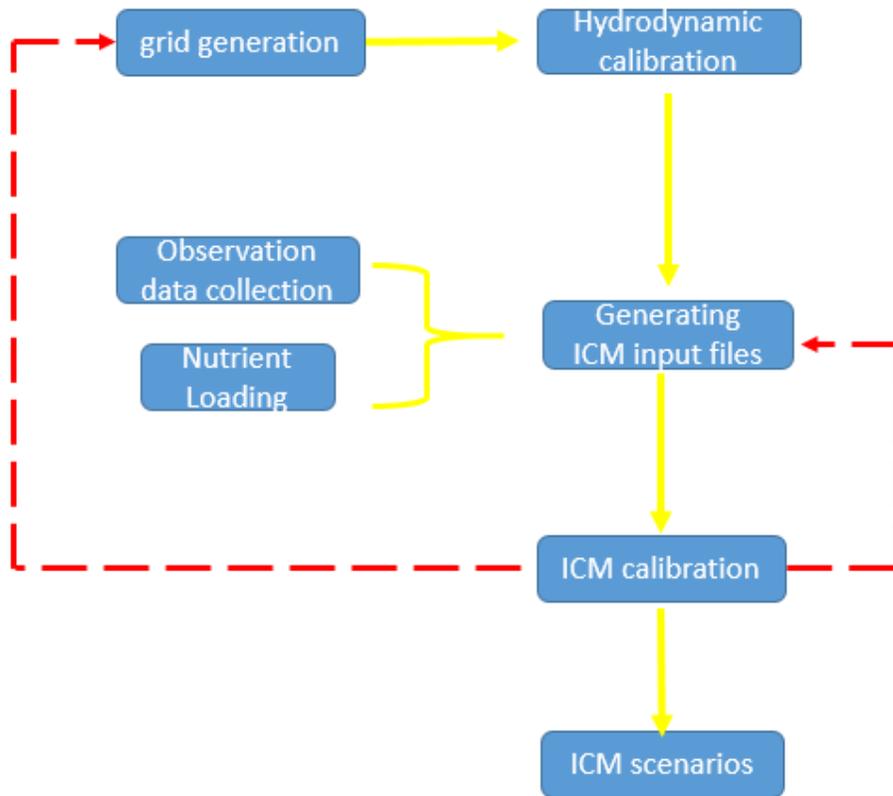


Figure 1. schematic for the ICM workflow

2 The coupling between SCHIMS and ICM

Figure 2 shows how ICM is coupled into SCHISM. The major subroutines in ICM mode was shown. In the model, the initialization includes: read in of ICM parameters, preprocessing of ICM variables (declaration and initialization) and pre-calculations. When SCHISM starts its loop of time, ICM kinetics (subroutine **ecosystem**) was invoked every time step. Since, the time scale of ecosystem processes O(hour) is generally larger than the time step of hydrodynamics O(minute), ICM module also provide an option to be invoked every **NDTWQ** time steps of hydrodynamics, where **NDTWQ** is a ICM parameter. For the current model, the ICM kinetics only take a small part of total computation time, which the physical transport is the big part. In the further model development, **NDTWQ** maybe a good way to improve model efficiency if large transport time step is allowed.

Below are some of the major subroutines in ICM along with a simple description for each.

ecosystem: main ICM routine

link_icm: link between ICM variables and SCHISM variable **tr_el**

Phyto: compute phytoplankton growth rates

calkwq: solve ICM mass balance equations

ph_calc: PH calculation

icm_init: ICM variable allocation and initialization.

WQinput: read time varying input for solar radiation, benthic fluxes, atmospheric loading.

read_icm_param: read parameters in icm.in. This is for water quality model

read_icm_param2: read spatially varying parameters

read_icm_sed_param: read sediment flux model parameters

sed_calc: calculate sediment flux; sub-models

link_sed_input: initialize sediment at the beginning of each step

link_sed_output: pass sediment fluxes to ICM

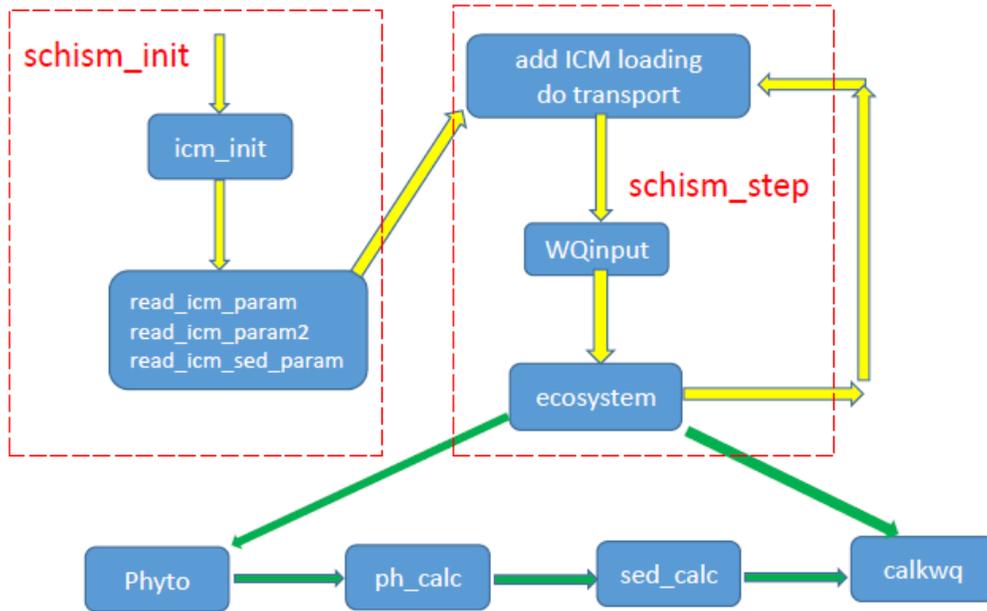


Figure 2. model flows for SCHISM and ICM

3 Variables in ICM

Table 1 shows 21 ICM variables in the water column including zooplankton, phytoplankton, organic carbon, nitrogen, phosphorus, silica, chemical oxygen demand and dissolved oxygen. All these variables are fully dynamically linked in the model. Sometimes, a simpler specification of zooplankton dynamics is preferred and ICM module provides such an option ($iZoo=0$). In this case, the zooplankton dynamics is skipped by the model. Instead, a simple predation parameter on phytoplankton was set and one can just specify zero zooplankton concentration. The first two variables are then useless and one can regard this as a 19 variables water quality model (ICM 19).

Please pay attention that in the ICM code, the variable name of DOC is **DOCA** and the variable name of DO is **DOC** as a legacy of previous ICM version.

Table 1. state variables in water column

Symbol	Parameter	Tracer Numbering	Unit
ZB1	1 st zooplankton	1	Mg/L
ZB2	2 nd zooplankton	2	Mg/L
PB _d (or PB1)	Diatom	3	Mg/L
PB _g (or PB2)	Green Algae	4	Mg/L
PB _c (or PB3)	Cyanobacteria	5	Mg/L
RPOC	Refractory Particulate Organic Carbon	6	Mg/L
LPOC	Labile Particulate Organic Carbon	7	Mg/L
DOC	Dissolved Organic Carbon	8	Mg/L
RPON	Refractory Particulate Organic Nitrogen	9	Mg/L
LPON	Labile Particulate Organic Nitrogen	10	Mg/L
DON	Dissolved Organic Nitrogen	11	Mg/L
NH ₄	Ammonium Nitrogen	12	Mg/L
NO ₃	Nitrate+Nitrite Nitrogen	13	Mg/L
RPOP	Refractory Particulate Organic Phosphorus	14	Mg/L
LPOP	Labile Particulate Organic Phosphorus	15	Mg/L
DOP	Dissolved Organic Phosphorus	16	Mg/L
PO _{4t}	Total Phosphate	17	Mg/L

SU	Particulate Biogenic Silica	18	Mg/L
SA	Available Silica	19	Mg/L
COD	Chemical Oxygen Demand	20	Mg/L
DO	Dissolved Oxygen	21	Mg/L

If pH module is invoked ($iPh=1$), additional four variables are added to account the pH model kinetics including total inorganic carbon, alkalinity, dissolved calcium and calcium carbonate. However, pH is not a state variable in the model. Instead, it is calculated using TIC and ALK based on the aquatic chemistry. The calculation of pH is a key process in pH model. In ICM model, a robust method was introduced and tested for the calculation. In addition, calcium species are included in this model as a buffer system. Please note that all initial and boundary conditions for these four additional pH model variables are needed if pH model is turned on. More information will be introduced about the preparation of these input files.

Table 2. variables of pH model in ICM

Symbol	Parameter	Tracer Numbering	Unit
TIC	Total Inorganic Carbon	22	Mg/L
ALK	Alkalinity	23	Mg[CaCO ₃]/L
CA	Dissolved Calcium	24	Mg[CaCO ₃]/L
CACO ₃	Calcium Carbonate	25	Mg[CaCO ₃]/L

4 Model Parameters

In the clean-up of ICM code in 2015-2016, some names are modified in order for readers to better recognize them. In addition, much effort was put on removing the unnecessary parameters and variables. However, most of the parameters in the present model are still standard ICM names. This section gives description about each parameter in parameter file `icm.in` and their use in the model. The parameters are grouped based on their functions on ICM variables.

4.1 Global Switches

- **iLight (int)**: methods for TSS calculation
iLight=1: $rKe=rKeC1*\exp(-rKeC2*Sal(k))$, this simple method is not recommended. rKe is the light extinction coefficient.
iLight=2: $rKe=rke0+rKeC2*Chl+rKeC3*TSS$; Here TSS is from sediment model. This method is most elegant, but needs good SED3D results.
iLight=3: $rKe=rke0+rKeC2*Chl+rKeC3*TSS$: Here TSS is related to Particulate Organic Carbon (POC) and PC2TSS.gr3 is needed in this case. In this case, $iTSS=1/2$ is used to specify a uniform/spatially varying coefficient.
- **jLight (int)**: choice for the formulation of phytoplankton light limitations. When **jLight=1**, a method described in (Chapra 1997) is used and one also can refer to the code in the model for the formulation. In the model, there is variable **rIs** (optimal light intensity) calculated based on the light intensities in the latest three days. If **jLight=2**, a more sophisticated method is used. This method is borrowed from (Cerco and Noel 2004) by specifying the initial slope of P-I curves. The second method is encouraged. This part is very important for the costal and estuarine ecosystem modeling and more tests are needed in the future to make this part more rigorous.
- **iSun (int)**: an old method used to specify model temperature in the ICM. Not used anymore.
- **iNPS (int)** and **iPS (int)**: flags for nonpoint and point load sources. These two options are the traditional ways of how watershed loading is added in the ICM code. These two options are not used in the present SCHISM+ICM model. However, options are still kept in the code for the future need. In the mass balance equation for each ICM state variable, these sources are included as variable names starting with a letter “W” in the code. For instance, **WLPOC** is used to represent nonpoint source, while **WPLPOC** is used for point source.
- **iSed (int)**: switch for sediment flux model (**iSed=1**). When evaluating the water quality processes, one can actually shut down sediment flux model with **iSed=0**. In this case, one can apply simple sediment flux by use **iBen=1** or **2** (see below). With these options, one

can better assess the kinetic processes in the water column and how they are related to the sediment fluxes.

- **iRea (int)**: option for surface DO reaeration. When **iRea=0**, the method described in (Park et al., 1995) is used. When **iRea=1**, the method described in (Cercio and Noel 2004) is used. The second method is preferred in the Chesapeake Bay application, which takes account the effects of temperature, salinity and wind speed.
- **iZoo (int)**: switch for zooplankton.
iZoo=1: add zooplankton dynamics (2 species) to the model. if **iZoo=0**, a simple formulation is used for phytoplankton predation, which follows the EFDC manual. If **iZoo=1**, then, zooplankton will eat phytoplankton and organic carbon (RPOC, LPOC and DOC). In the past, I prefer to use **iZoo=0** since zooplankton observation is not available in most cases and this simple predation simplifies the model. However, the choice is up to the user and one can use the default values as a start. Please note zooplankton variables always exist in the model when using **iZoo=0** option, which means all initial and boundary conditions for 2 zooplankton species are always needed. In the case when **iZoo=0**, one can just use “0” for all the initial and boundary conditions for zooplankton.
- **iPh (int)**: pH model switch
If **iPh=1**, PH model is invoked in ICM. Then, four additional variables should be taken into consideration when generating input files. Also, pH is not a ICM variables, but there is a S output option for pH in the SCHISM parameter files. More detail about how pH is modeled will be covered in the following section about pH model kinetics.
- **iAtm (int)**: flag for ICM atmospheric loading. For **iAtm=1**, a uniform loading is used for the entire domain. This option is now available for the code. Usually, this is the preferred option for atmospheric loading. Spatially varying loading (**iAtm=2**) is also possible for a very large domain. In this case, a little work is needed, just following the code for **iBen=2** (spatially varying benthic fluxes, see below). When **iAtm=1** or 2, input file **ICM_atm.th** is

needed. The format follows standard SCHISM *.th format and one can refer to the code for more details.

- **iBen (int)**: flag for specifying ICM benthic fluxes **iBen=0, 1 or 2**. When combined with sediment flux model (**iSed=1 and iBen≠0**), this option provides additional sediment fluxes. If sediment flux model is turned off, this parameter also provides a simple way to add sediment fluxes. When **iBen=1 or 2**, input file **ICM_ben.th** is needed. The format follows standard SCHISM *.th format and one can refer to the code for more details. If **iBen=0**, no additional sediment flux is applied. When **iBen=1**, a uniform sediment flux is used for all tracers. When **iBen=2**, a spatially varying sediment flux is used. Both options are now available in the current model. The option **iBen=1 or 2** is usually used when sediment flux model is turned off **iSed=0**. It gives a simple method to specify sediment fluxes to the water column. Basically, the flux rates of carbon, nitrogen, phosphorus, silica, chemical oxygen demand and oxygen are needed in the input files. Additionally, a temperature dependent coefficient is needed for each tracer to specify how the sediment flux changes with temperature. Usually, only nitrogen and phosphorus fluxes are needed. In this case, one can just use “0” for other tracers.
- **iRad (int)**: flag for solar radiation. At present, only uniform solar radiation specification (**iRad=1**) is allowed in the model. For spatially varying solar radiation **iRad=2**, a little coding work is needed and one can follow the method for **iBen=2**, which is very straightforward in the code. When **iRad=1**, the input file **ICM_rad.th** is needed. In this file, the daily radiation strength (**rIa** in the code) is needed. Additionally, the sunrise (**TU**) and sunset (**TD**) times in hours should be specified. The input should be in daily basis with a spacing in one day. Also, the solar radiation is in unit of ly/day (this is the legacy of traditional ICM). In the later, one can use other approach to improve this part. For example, in CoSiNE code, just relate solar radiation to the short wave radiation **srad** read in from sflux files.
- **iCheck (int)**: when **iCheck=1**, the code will output all ICM parameters for check.

- `iout_icm` (int) and `nspool_icm` (int): flag for ICM station outputs (`iout_icm=1`). This option is a very economical way to run the model, especially for experimenting scenarios. My experience is that outputting all 3D ICM variables is not necessary in many cases. It is also painful to process ICM results for complete 3D output as the amount of output maybe huge. I suggest this method for simple and quick diagnostics of the ICM model. Another advantage of this option is that you can output intermediate variables for analysis of the results, but it need you to code accordingly. The coding is very simple and one can just add any variable you want to output channel 410. This method is also applied in the SCHISM+CoSiNE model, which is tested vigorously in CoSiNE model. However, testing in the ICM is still not sufficient. Please let me know if you find any problem when using this option. When `iout_icm=1`, `nspool_icm` is needed to specify the time steps for output.

4.2 Other Global Parameters

This part is for some parameters that can be uniform or spatially varying. In the ICM code, these parameters are read in from subroutine `read_icm_param2`.

- `iWS` (int), `WSRP` (double), `WSLP` (double), `WSPB1` (double), `WSPB2` (double), `WSPB3` (double), and `WSSED` (double)

`iWS` is the flag for uniform or spatially varying settling velocities. If `iWS=1`, uniform settling velocities are used for Refractory Particulate Organic Matters (RPOM), Refractory Larticulate Organic Matters (LPOM), Diatom, Green Algae, Cyanobacteria, and TSS, and their velocities are read in from parameters: `WSRP`, `WSLP`, `WSPB1`, `WSPB2`, `WSPB3`, `WSSED`. If `iWS=2`, spatial varying velocities are used and are read in from `settling.gr3`. The format is similar to `*gr3` files, but more values are appended each line. Below is the format.

```
read(31,*)ip,xtmp,ytmp,tWSRP,tWSLP,tWSPB1,tWSPB2,tWSPB3
```

Based on personal experience in Chesapeake Bay, settling velocities are key parameters for the ecosystem modeling in estuarine. Choosing appropriate settling velocities are important and in many cases sensitivities tests are needed. Normally, diatom has the largest settling velocity, and cyanobacteria has the smallest settling velocity (or even zero settling velocity).

- `iTurb` (int) and `Turb` (double):
When `iTurb=1` or `2`, specify uniform/spatially varying background light extinction coefficient. If `iTurb=1` is used, one should provide value for parameter `Turb`. Otherwise if `iTurb=2` is used, one should provide input file `Turb.gr3`.
- `iWRea` (int) and `WRea` (double)
If `iWRea=1` or `2`, specify uniform/spatially varying background coefficient for wind-induced DO reaeration. If `iWRea=1` is used, one should provide value of `WRea`. Otherwise if `iWRea=2` is used, one should provide input file `WRea.gr3`.

- **iTSS** (int) and **PC2TSS** (double)

If **iTSS**=1 or 2, specify uniform or spatially varying coefficient for the relation between TSS and POC when **iLight**=3 is used. It is used to estimate TSS based on modeled POC concentration (RPOC+LPOC). If **iTSS**=1, one should provide the value of **PC2TSS**. Otherwise if **iTSS**=2 is used, one should provide input file **PC2TSS.gr3**. Here, the relation coefficient between TSS and POC are often obtained from the linear regression between TSS and POC observations. This is a cheap way in estimating TSS instead of using full-fledged 3D sediment transport model. In many cases when there exists a good relationship between TSS and POC, the results are not bad. To make this method more complete, one can also use formulation $TSS=a+b*POC$ where the intersection “a” represents the inorganic parts of TSS.

4.3 Parameters: Zooplankton

When **iZoo**=1, zooplankton parameters are needed for zooplankton dynamics. In ICM, there are two zooplankton species: copepod and others (or mesozooplankton and microzooplankton) depending on their sizes. Parameters are needed to specify their predation, basal metabolism, and mortality. Zooplankton can graze on each other (normally mesozooplankton eats microzooplankton), carbon, and phytoplankton. Therefore, there are 8 kinds of prey. Some tests have been done before on the zooplankton dynamics before, but are limited and not rigorous. Overall, it seems that the zooplankton behaves normally, but it needs more tests in future applications. With the new option **iout_icm**=1, it adds more convenience for this kind of tests.

1. **GZM**(**i**=1:8, **j**=1:2): zooplankton predation rate (day^{-1}). The first index is prey **i** and the second corresponds to the zooplankton species **j**.
2. **rKhGE**(**i**=1:8, **j**=1:2): half-saturation concentration of prey **i** by zooplankton **j** (Mg/L).
3. **PPC**(**i**=1:8, **j**=1:2): preference of zooplankton **j** go graze on prey **i**. If **PPC**(**i,j**)=0, it means that zooplankton **j** does not graze on prey **i**.
4. **BMZR**(**j**=1:2): basal metabolism rate of zooplankton **j** (day^{-1}) at temperature **TBZ**(**j**).
5. **DRZ**(**j**=1:2): death rate of zooplankton **j** (day^{-1}).
6. **TGZ**(**j**=1:2): optimal temperature for the growth of zooplankton **j** ($^{\circ}\text{C}$).

7. **rKTGZ1(j=1:2)**: effect of temperature on the growth of zooplankton **j** when temperature is above **TGZ(j)** ($1/^\circ\text{C}^2$).
8. **rKTGZ1(j=1:2)**: effect of temperature on the growth of zooplankton **j** when temperature is lower than **TGZ(j)** ($1/^\circ\text{C}^2$).
9. **TBZ(j=1:2)**: reference temperature for the basal metabolism of zooplankton **j** ($^\circ\text{C}$).
10. **rKTBZ(j=1:2)**: effect of temperature on the metabolism of zooplankton **j** ($1/^\circ\text{C}$).
11. **RZ(j=1:2)**: proportional rate of higher trophic predation (eg. fish) rate on zooplankton **j** ($\text{Mg}\cdot\text{L}^{-1}\cdot\text{day}^{-1}$) to the total biomass of zooplankton and phytoplankton. The assumption is that the biomass of higher trophic level is proportional of the total biomass of zooplankton and phytoplankton.
12. **Eff**: assimilation efficiency.
13. **RF**: respiration of grazing. This is the part of energy consumed when zooplankton grazes.
14. **Pf**: proportional rate of higher trophic predation (eg. fish) rate on phytoplankton ($\text{Mg}\cdot\text{L}^{-1}\cdot\text{day}^{-1}$) to the total biomass of zooplankton and phytoplankton. The assumption is that the biomass of higher trophic level is proportional of the total biomass of zooplankton and phytoplankton.

4.4 Parameters: Phytoplankton

There are 3 phytoplankton species: Diatom, green algae and cyanobacteria. Phytoplankton does not interact with each other. The same kinds of parameters are used to characterize each phytoplankton species. The different behaviors of each species are dependent on the parameter values except two instances: a). available silica affects diatom growth and b). salinity limits freshwater cyanobacteria growth. All these parameters are in the **float** format.

1. **GPM(i=1:3)**: maximum growth rate of phytoplankton **i** under optimal conditions (day^{-1}). Normally in Chesapeake Bay estuary, values around $2-3 \text{ day}^{-1}$ are used.
2. **BMPR(i=1:3)**: basal metabolism rate of phytoplankton **i** at temperature **TBP(i)** (day^{-1}).
3. **PRR(i=1:3)**: predation rate on phytoplankton **i** at temperature **TBP(i)** (day^{-1}). This parameter is used for simple predation formulation when zooplankton dynamics are turned

off $iZoo=0$. For a simple case, this greatly reduce the complexity of the ICM model as especially when there is no observation to justify the zooplankton parameterization.

4. **TBP**($i=1:3$): reference temperature for basal metabolism (also predation rate) of phytoplankton i ($^{\circ}\text{C}$).
5. **TGP**($i=1:3$): optimal temperature of the growth of phytoplankton i ($^{\circ}\text{C}$).
6. **rKTGP1**($i=1:3$): effect of temperature on the growth of phytoplankton i when temperature is above TBP(i) ($1/^{\circ}\text{C}^2$).
7. **rKTGP2**($i=1:3$): effect of temperature on the growth of phytoplankton i when temperature is below TBP(i) ($1/^{\circ}\text{C}^2$).
8. **rKTBP**($i=1:3$): effect of temperature on the metabolism (also predation rate) of phytoplankton i ($1/^{\circ}\text{C}$).
9. **CChl**($i=1:3$): fixed carbon to chlorophyll ratio for phytoplankton i in the ecosystem model ($\text{g}[\text{C}]/\text{Mg}[\text{Chl}]$). Typically, one can use 0.059 for all species in Chesapeake Bay. Right now, this model does not have a way to dynamically calculate the ratio. One can change the ratio accordingly based on the specific application.
10. **rKhN**($i=1:3$): half-saturation constant for nitrogen uptake of phytoplankton i (Mg/L).
11. **rKhP**($i=1:3$): half-saturation constant for phosphorus uptake of phytoplankton i (Mg/L).
12. **rIm**($i=1:3$): a reference minimum light intensity that phytoplankton i can grow (ly/day).
This value is used only for $j\text{Light}=1$.
13. **alpha_PB**($i=1:3$): the initial slope of P-I curve for phytoplankton i .
14. **rKhS**: half-saturation constant for silica uptake of diatom (Mg/L).
15. **ST**: reference salinity for salinity toxicity of cyanobacteria (PPT).
16. **rKeC1** and **rKeC2**: Two parameters used to specify light attenuation by relating it to salinity when $i\text{Light}=1$. This method is not encouraged. It is just a legacy of previous ICM model.
17. **Dopt**: depth of optimal light intensity for phytoplankton growth (m).

4.5 Parameters: Carbon

1. **FCRPZ, FCLPZ, FCDPZ**: partition coefficients how zooplankton matter goes to RPOC, LPOC and DOC. The zooplankton matter is generated in three processes: a). higher trophic level grazes on zooplankton, b). zooplankton grazes on each other and c). death of zooplankton. Overall, $FCRPZ+FCLPZ+FCDPZ=1$.
2. **FCDZ(j=1:2)**: fraction of basal metabolized carbon by zooplankton **j** to DOC. Please pay attention to that another part of basal metabolized zooplankton carbon which depends on the oxygen concentration can also goes into the DOC pool. The rest goes into the DIC pool.
3. **rKHRZ(j=1:2)**: half saturation of dissolved oxygen for zooplankton **j** excretion of DOC (Mg/L).
4. **FCRP, FCLP, FCDP**: partition coefficients how phytoplankton matter goes to RPOC, LPOC and DOC. The phytoplankton matter is generated in two processes: a). higher trophic level grazes on phytoplankton and b). zooplankton grazes phytoplankton. Overall, $FCRP+FCLP+FCDP=1$.
5. **FCD(i=1:3)**: fraction of basal metabolized carbon by phytoplankton **i** into DOC. Please pay attention to that another part of basal metabolized phytoplankton carbon which depends on the oxygen concentration can also goes into the DOC pool. The rest goes into the DIC pool.
6. **rKHR1, rKHR2, and rKHR3**: half saturation of dissolved oxygen for the excretion of DOC of three phytoplankton species (Mg/L).
7. **rKRC and rKLC**: minimum dissolution rate for RPOC and LPOC (day^{-1}). The end product goes into DOC pool.
8. **rKDC**: minimum respiration rate of DOC (day^{-1}). The end product goes into DIC pool
9. **rKRCalg, rKLCalg, and rKDCalg**: effect of phytoplankton biomass on the dissolution of RPOC and LPOC, and the respiration of DOC. The assumption is that phytoplankton biomass can represent the degree of heterotrophic activity.
10. **TRHDR**: reference temperature for hydrolysis of POM ($^{\circ}\text{C}$)
11. **TRMNL**: reference temperature for mineralization of DOM ($^{\circ}\text{C}$)
12. **rKTHDR**: effect of temperature on hydrolysis of POM ($^{\circ}\text{C}$)

13. **rKTMNL**: effect of temperature on mineralization of DOM (°C)
14. **rKHORDO**: half-saturation concentration of DO for oxic respiration (Mg/L)
15. **rKHDNn**: half-saturation concentration of nitrate for denitrification (Mg/L)
16. **AANOX**: ratio of denitrification rate to oxic DOC respiration rate. This coefficient is used to relate denitrification rate to DOC respiration rate.

4.6 Parameters: Nitrogen

1. **FNRPZ**, **FNLpz**, **FNDpz** and **FNIPZ**: partition coefficients how zooplankton matter goes to RPON, LPON, DON and NH₄. The zooplankton matter is generated in three processes: a). higher trophic level grazes on zooplankton, b). zooplankton grazes on each other and c). death of zooplankton. Overall, **FNRPZ+FNLpz+FNDpz+FNIPZ=1**.
2. **FNRZ(j=1:2)**, **FNLZ(j=1:2)**, **FNDZ(j=1:2)**, and **FNIZ(j=1:2)**: fraction of basal metabolized nitrogen of zooplankton **j** to RPON, LPON, DON and NH₄. Overall, **FNRZ+FNLZ+FNDZ+FNIZ=1**.
3. **ANCZ(j=1:2)**: nitrogen to carbon ratio for zooplankton **j**.
4. **FNRp**, **FNLp**, **FNDp** and **FNIP**: partition coefficients how phytoplankton matter goes to RPON, LPON, DON and NH₄. The phytoplankton matter is generated in two processes: a). higher trophic level grazes on phytoplankton and b). zooplankton grazes phytoplankton. Overall, **FNRp+FNLp+FNDp+FNIP=1**.
5. **ANDC**: mass of nitrate nitrogen reduced per mass of dissolved organic carbon oxidized (g [N] per g[C])
6. **FNR(i=1:3)**, **FNL(i=1:3)**, **FND(i=1:3)** and **FNI(i=1:3)**: fraction of basal metabolized nitrogen of phytoplankton **i** into RPON, LPON, DON and NH₄. Overall, **FNR+FNL+FND+FNI=1**.
7. **ANC(i=1:3)**: nitrogen to carbon ratio for phytoplankton **i**.
8. **rKRN** and **rKLN**: minimum dissolution rate for RPON and LPON (day⁻¹). The end product goes into DON pool.
9. **rKDN**: minimum mineralization rate of DON (day⁻¹). The end product goes into NH₄ pool.

10. **rKR_{Nalg}**, **rKL_{Nalg}**, and **rKD_{Nalg}**: effect of phytoplankton biomass on the dissolution of RPON and LPON, and the mineralization of DON. The assumption is that phytoplankton biomass can represent the heterotrophic activity.
11. **TN_{it}**: optimal temperature for nitrification (°C)
12. **rKN_{it1}** and **rKN_{it2}**: temperature effect on nitrification rate when temperature is below or above **TN_{it}** (°C⁻²)

4.7 Parameters: Phosphorus

1. **FPRPZ**, **FPLPZ**, **FPDPZ** and **FPIPZ**: partition coefficients how zooplankton matter goes to RPOP, LPOP, DOP and PO₄. The zooplankton matter is generated in three processes: a). higher trophic level grazes on zooplankton, b). zooplankton grazes on each other and c). death of zooplankton. Overall, **FPRPZ+FPLPZ+FPDPZ+FPIPZ=1**.
2. **FPRZ(j=1:2)**, **FPLZ(j=1:2)**, **FPDZ(j=1:2)**, and **FPIZ(j=1:2)**: fraction of basal metabolized phosphorus of zooplankton **j** to RPOP, LPOP, DOP and PO₄. Overall, **FPRZ+FPLZ+FPDZ+FPIZ=1**.
3. **ANCZ(j=1:2)**: phosphorus to carbon ratio for zooplankton **j**.
4. **FPRP**, **FPLP**, **FPDP** and **FPIP**: partition coefficients how phytoplankton matter goes to RPOP, LPOP, DOP and PO₄. The phytoplankton matter is generated in two processes: a). higher trophic level grazes on phytoplankton and b). zooplankton grazes phytoplankton. Overall, **FPRP+FPLP+FPDP+FPIP=1**.
5. **FPR(i=1:3)**, **FPL(i=1:3)**, **FPD(i=1:3)** and **FPI(i=1:3)**: fraction of basal metabolized phosphorus of phytoplankton **i** into RPOP, LPOP, DOP and PO₄. Overall, **FPR+FPL+FPD+FPI=1**.
6. **APC(i=1:3)**: phosphorus to carbon ratio for phytoplankton **i**.
7. **rKPO_{4p}**: empirical coefficient relating phosphate sorption to total suspended solid (per mg/L).
8. **rKRP** and **rKLP**: minimum dissolution rate for RPOP and LPOP (day⁻¹). The end product goes into DOP pool.

9. **rKDP**: minimum mineralization rate of DOP (day^{-1}). The end product goes into PO₄ pool.
10. **rKR_{Nalg}**, **rKL_{Nalg}**, and **rKD_{Nalg}**: effect of phytoplankton biomass on the dissolution of RPON and LPON, and the mineralization of DON. The assumption is that phytoplankton biomass can represent the heterotrophic activity.

4.8 Parameters: Silica

1. **FSPPZ**, and **FSIPZ**: partition coefficients how zooplankton matter goes to SU and SA. The zooplankton matter is generated in three processes: a). higher trophic level grazes on zooplankton, b). zooplankton grazes on each other and c). death of zooplankton. Overall, **FSPPZ+FSIPZ** =1.
2. **FSRZ(j=1:2)**, **FSIZ(j=1:2)**: fraction of basal metabolized silica of zooplankton **j** to SU and SA. Overall, **FSRZ+FSIZ**=1.
3. **ASCZ(j=1:2)**: silica to carbon ratio for zooplankton **j**.
4. **FSPP**, **FSIP**: partition coefficients how diatom matter goes to SU and SA. The diatom matter is generated in two processes: a). higher trophic level grazes on diatom and b). zooplankton grazes diatom. Overall, **FSPP+FSIP**=1.
5. **FSPd**, **FSId**: fraction of basal metabolized silica of diatom into SU and SA. Overall, **FSPd+FSId**=1.
6. **ASCd**: silica to carbon ratio for diatom.
7. **rKSAP**: empirical coefficient relating available silica sorption to total suspended solid (per mg/L).
8. **rKSU**: dissolution rate of particulate biogenic silica at TRSUA (day^{-1})
9. **TRSUA**: reference temperature for dissolution of particulate biogenic silica ($^{\circ}\text{C}$)
10. **rKTSUA**: effect of temperature on dissolution of particulate biogenic silica ($^{\circ}\text{C}^{-1}$)

4.9 Parameters: COD and dissolved oxygen

1. **rKHCOD**: half saturation constant of dissolved oxygen required for the oxidation of chemical oxygen demand ($\text{mg}[\text{O}_2]/\text{L}$)

2. **rKCD**: oxidation rate of chemical oxygen demand at **TRCOD** (day^{-1})
3. **TRCOD**: reference temperature for oxidation of COD ($^{\circ}\text{C}$)
4. **KTCOD**: effect of temperature on oxidation of COD ($^{\circ}\text{C}^{-1}$)
5. **AOC**: dissolved oxygen to carbon ratio in respiration ($\text{g } [\text{O}_2] \text{ per g } [\text{C}]$)
6. **AON**: mass of dissolved oxygen consumed per unit mass of ammonium nitrogen nitrified ($\text{g } [\text{O}_2] \text{ per g}[\text{N}]$)
7. **rKro**: reaeration coefficient (day^{-1}) for **iRea=0**
8. **rKTr**: constant for temperature adjustment of DO reaeration rate when **iRea=0**

5 ICM Input files

Besides Hydrodynamic input file, ICM needs additional inputs. Here, I lists some inputs file that I usually used in the past. Choosing appropriate values for these input files is as equally important as tuning model parameters. The main reason is that there exists big uncertainty for water quality model. Therefore, one should pay attentions to generating ICM inputs. One should consider each variable as carefully as possible. Please refer to observation data often and make reasonable assumption for missing variables. Iteration process may be needed also.

- 1) Initial condition: **hotstat.nc** (or **hotstart.in**) or **ICM_hvar_#.ic**

Normally, I would suggest one use **hotstart.nc** for initial condition since it is more comprehensive. For ICM variables in the water column, one can interpolate water quality observation data to get spatially varying inputs. For some variables not available, one should make reasonable assumption by relating it to some known variables. For example, one can relate $\text{RPN} = 0.5 * \text{DON}$ if RPN information is unknown. Here 0.5 is an assumption ratio, probably obtained from the relationship between RPN and DON observations. Also, $\text{COD} = 0.0$ is generally used for initial condition. For phytoplankton ($\text{PB}_d, \text{PB}_g, \text{PB}_c$), there are two points one should pay attention to. First, CHLA is usually measured in unit of ($\mu\text{g/L}$), but the unit in ICM model is Mg/L . Therefore, a carbon to chlorophyll ratio should be used for the conversion. In the past, I usually use 0.059. Second, total CHLA should be partitioned into three parts. Normally, diatom grows at lower temperature and it should have a bigger proportion if

the model starts at beginning of the year. The principle also applies to the boundary condition. For sediment initial concentration, please refers to the default initial values in [icm_sed.in](#). These values are good choices for start. After several years running and the model adjusting to a quasi-equilibrium state, one can save the condition at the end of year for the final initial condition. Of course, one can also use [ICM_hvar_#.ic](#) for cold start.

2). Boundary Condition: [ICM_3D.th](#) and ICM Nudging file: [ICM_nu.in](#)

Based on my experience, one should use [ICM_3D.th](#) for costal ocean boundary condition since it is often lack of observation. It is better to let the model adjust itself if there is an uncertainty. However, inside the estuary (eg. inside Chesapeake Bay), one can generate [ICM_nu.in](#) based on observation data to ensure fixed values that match the boundary.

3). Atmospheric Loading: [ICM_atm.th](#)

The format of this file is standard SCHISM *.th input. However, only these variables should be added in this file (RPOC, LPOC, DOC, RPON, LPON, DON, NH4, NO3, RPOP, LPOP, DOP, PO4, SU, SA, COD, DO). Generally, nitrogen and phosphorus atmospheric loading are needed. One can use zeros for other values.

4). Photosynthetically Active Radiation (PAR): [ICM_rad.th](#)

The format of this file is:

```
read(403,*) time, rad, TU, TD
```

where [rad](#) is the daily maximum radiation, [TU](#) and [TD](#) are local sunrise and sunset times in hour. In the model, a sine curve is used to represent daily radiation variation. This part of code can be improved by relating SCHISM [srad](#) to PAR for simplicity, which is also adopted in SCHISM+CoSiNE model. I think this is a better way for solar radiation.

5). Sediment Flux Input: [ICM_ben.th](#)

This option is to replace sediment flux model. One can specify sediment fluxes for these variables (RPOC, LPOC, DOC, RPON, LPON, DON, NH4, NO3, RPOP, LPOP, DOP, PO4, SU, SAt, COD, DO). You can use uniform values or spatially varying values. Please refer to

the code for its format. Also, please note temperature dependent coefficients for sediment fluxes should be specified. If sediment flux model is used, one can use zero values, or `iSed=0` to exclude it. Otherwise, `ICM_ben.th` provides additional sediment fluxes.

6). Loading inputs: `vsource.th` and `msource.th`

Right now, all loading inputs to the model are added using SCHISM `if_source=1` option. This includes both non-point and point sources loading. If both of them are provided, please add them together since SCHISM+ICM does not differentiate them. A concern is where to add the loading. For example, if the loading is provided as watershed-based format. One should consider partitioning the load to certain grid elements. In Chesapeake Bay, you can refer to the script I provided to Ping Wang. Another issue is that original ICM model loading is usually mass oriented and is added as mass. Sometimes, the actual nutrient loading concentrations are abnormally high and unrealistic. However, the nutrient loading in SCHISM+ICM is added as concentrations. They should be consistent with volume source. Please double check the input files if EPA loading is used.

7). TSS calculation: `PC2TSS.ic`

This is the coefficient between TSS and POC. Since ICM does not simulate TSS, one can relate TSS to POC, where the coefficient is provided in `PC2TSS.ic`. You can obtain this coefficient using regression between POC to TSS. In Chesapeake Bay, this is a very economical way and the result is not bad in many cases.

8). Settling velocity: `settling.gr3`

In the model, one can use uniform settling velocity `iWS=1` for RPOM, LPOM, and phytoplankton species. However, `settling.gr3` provides a better way. One can use spatially varying settling velocity. For example, one can use small values in shallow region and large values in deep regions. This option seems useful based on my experience in Chesapeake Bay. Also, Carl Cerco uses different velocities in different regions in his latest Chesapeake Bay Model.

9). Parameter files: `icm.in` and `icm_sed.in`

`icm.in` is the parameter file for water column dynamics and most of global switches are also included in this file. `icm_sed.in` is parameter file for sediment flux module. There are many parameters that can influence water quality model simulation. For phytoplankton, the most sensitive parameters are growth rates (`GPM`), settling velocity (`WSPB1`, `WSPB2`, `WSPB3`), optimal temperature (`TGP`). For tuning nutrient species, one should analyze the results based on the kinetic equations to identify the big drivers. Then, adjust the corresponding parameters. Often, the partitioning coefficients are important for determining the concentration of nutrient species. Also, please note, the parameters are organized in groups and one can refer to all the parameters related to certain species accordingly. Along with ICM code, sample files `icm.in.sample` and `icm_sed.in.sample` are provided. One can use them as a start. The values in these files are typical values I used in the past and many of them are literature values. In addition, references (Park et al., 1995; Cerco and Noel 2004) are important manuals and one can refer to them for parameter adjustment.

6 Kinetics

In this section, we will describe the kinetics of ICM model in the water column. Right now, the zooplankton kinetics are not included (referred as ICM 19). The inclusion of zooplankton dynamics (referred as ICM 21) adds much complexity for the equations. Here, simple formation of predation of phytoplankton is first introduced. Later, we will add a section separately to describe the new equations with zooplankton species. Also, we will gradually add description about the sediment fluxes model. For the time being, one can refer to (Park, Kuo et al. 1995). For the pH model, we give out the related equations.

6.1 ICM 19

6.1.1 Phytoplankton

There are 3 phytoplankton (algal) groups in our model including diatom, green algae and cyanobacteria. The kinetics of phytoplankton includes growth, metabolism, predation, settling and external loads. The growth depends on nutrient, light and temperature. The growth of diatom also

depends on silica concentration. Additionally, salinity affects cyanobacteria growth. For metabolism rate and predation rate, they are largely influenced by temperature.

$$\frac{\partial PB_x}{\partial t} = (P_x - BMP_x - PR_x)PB_x + \frac{\partial(W S_x \cdot PB_x)}{\partial z} + \frac{WB_x}{V} \quad (1)$$

$$P_x = \begin{cases} PM_x \cdot f_1(N) \cdot f_2(I) \cdot f_3(T), & \text{for diatom and green alage} \\ PM_x \cdot f_1(N) \cdot f_2(I) \cdot f_3(T) \cdot f_4(S), & \text{for cyanobacteria} \end{cases} \quad (2)$$

$$f_1(N) = \begin{cases} \min\left(\frac{NH4 + NO3}{KHN_x + NH4 + NO3}, \frac{PO4_d}{KHP_x + PO4_d}\right), & \text{for green alage and cyanobacteria} \\ \min\left(\frac{NH4 + NO3}{KHN_x + NH4 + NO3}, \frac{PO4_d}{KHP_x + PO4_d}, \frac{SA_d}{KHS + SA_d}\right), & \text{for diatom} \end{cases} \quad (3)$$

$$f_2(I) = \frac{2.718 \cdot (e^{-\alpha_T} - e^{-\alpha_B})}{Ke \cdot \Delta z}, \quad \alpha_T = \frac{I_0}{(I_S)_x} \cdot e^{-Ke \cdot (H + \Delta z)}, \quad \alpha_B = \frac{I_0}{(I_S)_x} \cdot e^{-Ke \cdot H} \quad (4)$$

$$Ke = Ke_b + Ke_{TSS} \cdot TSS + Ke_{chl} \cdot \sum_x \left(\frac{PB_x}{cchl_x} \right) \quad (5)$$

$$f_3(T) = \begin{cases} e^{-KTG1_x \cdot (T - TM_x)^2}, & \text{if } T \leq TM_x \\ e^{-KTG2_x \cdot (TM_x - T)^2}, & \text{if } T > TM_x \end{cases} \quad (6)$$

$$f_4(S) = \frac{STOX^2}{STOX^2 + S^2} \quad (7)$$

$$BMP_x = BMR_x \cdot e^{KTB_x(T - TR_x)} \quad (8)$$

$$PR_x = PRR_x \cdot e^{KTB_x(T - TR_x)} \quad (9)$$

PB_x: algal biomass of algal species x (mg[C]/l)

t: time (day)
 P_x : production rate of algal group x (day^{-1})
 BM_x : metabolism rate of algal group x (day^{-1})
 PR_x : predation rate of algal group x (day^{-1})
 P_x : production rate of algal group x (day^{-1})
 WS_x : settling velocity of algal group x (m day^{-1})
 WB_x : external loads of algal group x (g [C] day^{-1})
 V: cell volume (m^3)
 PM_x : maximum growth rate under optimal conditions of algal group x (day^{-1})
 $f_1(\text{N})$: effect of nutrients on growth rate ($0 \leq f_1 \leq 1$)
 $f_2(\text{I})$: effect of light on growth rate ($0 \leq f_2 \leq 1$)
 $f_3(\text{T})$: effect of temperature on growth rate ($0 \leq f_3 \leq 1$)
 $f_4(\text{S})$: effect of salinity on growth rate for cyanobacteria ($0 \leq f_4 \leq 1$)
 KHN_x : half-saturation constant for algal nitrogen uptake (mg [N]/L)
 KHP_x : half-saturation constant for algal phosphorus uptake (mg [P]/L)
 KHS : half-saturation constant for diatom silica uptake (mg [Si]/L)
 $PO4_d$: dissolved phosphate concentration (mg [P]/L)
 SA_d : dissolved silica concentration (mg [Si]/L)
 Ke : light extinction coefficient (m^{-1})
 H: layer depth from water surface (m)
 Δz : layer thickness (m)
 I_0 : light intensity at water surface (langleys day^{-1})
 $(I_s)_x$: optimal light intensity for algal group x (langleys day^{-1})
 Ke_b : light extinction for background (m^{-1})
 Ke_{TSS} : light extinction coefficient for total suspended solid concentration (m^{-1} per mg/L)
 TSS: total suspended solid concentration (mg/L)
 Ke_{chl} : light extinction coefficient for total suspended solid concentration (m^{-1} per mg/L)
 $cchl_x$: carbon to chlorophyll ratio for algal group x (g[C] per mg[Chl])
 T: water temperature ($^{\circ}\text{C}$)
 TM_x : optimal temperature for algal growth for algal group x ($^{\circ}\text{C}$)
 $KTG1_x$: effect of temperature below TM_x on growth for algal group x ($^{\circ}\text{C}^{-2}$)

KTG_{2x}: effect of temperature above TM_x on growth for algal group x (°C⁻²)

STOX: salinity at which cyanobacteria growth is halved (ppt)

S: salinity (ppt)

BMR_x: metabolism rate at TR_x for algal group x (day⁻¹)

KTB_x: effect of temperature on metabolism for algal group x (°C⁻¹)

TR_x: reference temperature for metabolism for algal group x (°C)

PRR_x: predation rate at TR_x for algal group x (day⁻¹)

6.1.1.1 Light limitation for jLight=2

This section summarizes the formulation for the light limitation on phytoplankton growth in the ICM for jLight=2. Currently, this is the preferred method.

1). In the model, it first converts the short-wave solar radiation (W/m²) from the SCHISM surface forcing into the light intensity (Einstein/m²/day) in the ICM water quality model. The following equations are related to the conversion assuming the wavelength is $\lambda = 550 \text{ nm}$.

$$1 \text{ Einstein} = 6.022 \times 10^{23} \text{ photons} \quad (10)$$

$$\begin{aligned} \frac{1 \text{ Einstein}}{\text{m}^2 \cdot \text{day}} &= \frac{6.022 \times 10^{23} \times (h\nu)}{\text{m}^2 \cdot 86400\text{s}} = \frac{6.022 \times 10^{23} \times \left(\frac{hc}{\lambda}\right)}{\text{m}^2 \cdot 86400\text{s}} \\ &= \frac{6.022 \times 10^{23} \times (6.626 \times 10^{-34} \text{ J} \cdot \text{s}) \times \left(3 \times 10^8 \frac{\text{m}}{\text{s}}\right)}{\text{m}^2 \cdot 86400\text{s} \cdot (550 \times 10^{-9} \text{ m})} \\ &= 2.5191 \frac{\text{W}}{\text{m}^2} \end{aligned} \quad (11)$$

Therefore,

$$1 \frac{\text{W}}{\text{m}^2} = 0.397 \frac{\text{Einstein}}{\text{m}^2 \cdot \text{day}} \quad (12)$$

2). This part is about the formulation for light limitation (The 2010 Chesapeake Bay Eutrophication Model, Cerco 2010). The light limitation factor is

$$f_2(I) = \frac{I}{\sqrt{I^2 + IK^2}} \quad (13)$$

$$IK = \frac{P}{\alpha} \quad (14)$$

I : irradiance ($E \cdot m^{-2} \cdot day^{-1}$)

IK : reference irradiance ($E \cdot m^{-2} \cdot day^{-1}$)

P : photosynthetic rate ($g[C] \cdot g^{-1}[Chl] \cdot day^{-1}$)

α : initial slope between production and irradiance ($g[C] \cdot g^{-1}[Chl] \cdot E^{-1} \cdot m^2$)

6.1.2 Carbon

There are 3 carbon species in our model including refractory particulate organic carbon (RPOC), labile particulate organic carbon (LPOC), and dissolved organic carbon (DOC). For particulate organic carbon, the source is from the phytoplankton predation, while the loss includes hydrolysis and settling of particulate organic carbon. For dissolved organic carbon, the source includes phytoplankton metabolism, predation and hydrolysis of particulate organic carbon, while the loss includes heterotrophic respiration and denitrification.

$$\frac{\partial RPOC}{\partial t} = \sum_x FCRP \cdot PR_x \cdot B_x - K_{RPOC} \cdot RPOC + \frac{\partial}{\partial z} (WS_{RP} \cdot RPOC) + \frac{WRPOC}{V} \quad (15)$$

$$\frac{\partial LPOC}{\partial t} = \sum_x FCLP \cdot PR_x \cdot B_x - K_{LPOC} \cdot LPOC + \frac{\partial}{\partial z} (WS_{LP} \cdot LPOC) + \frac{WLPOC}{V} \quad (16)$$

$$\begin{aligned} \frac{\partial DOC}{\partial t} = \sum_x \left\{ \left[FCD_x + (1 - FCD_x) \frac{KHR_x}{KHR_x + DO} \right] BM_x + FCDP \cdot PR_x \right\} \cdot B_x \\ + K_{RPOC} \cdot RPOC + K_{LPOC} \cdot LPOC - K_{HR} \cdot DOC - Denit \cdot DOC + \frac{WDOC}{V} \end{aligned} \quad (17)$$

$$K_{RPOC} = \left(K_{RC} + K_{RCalg} \cdot \sum_x B_x \right) \cdot e^{KT_{HDR}(T - TR_{HDR})} \quad (18)$$

$$K_{LPOC} = \left(K_{LC} + K_{LCalg} \cdot \sum_x B_x \right) \cdot e^{KT_{HDR}(T-TR_{HDR})} \quad (19)$$

$$K_{HR} = \frac{DO}{KHOR_{DO} + DO} K_{DOC} \quad (20)$$

$$K_{DOC} = \left(K_{DC} + K_{DCalg} \cdot \sum_x B_x \right) \cdot e^{KT_{MNL}(T-TR_{MNL})} \quad (21)$$

$$Denit = \frac{KHOR_{DO}}{KHOR_{DO} + DO} \cdot \frac{NO3}{KHDN_N + NO3} AANOX \cdot K_{DOC} \quad (22)$$

FCRP: fraction of predated phytoplankton carbon produced as refractory particulate organic carbon

FCLP: fraction of predated phytoplankton carbon produced as labile particulate organic carbon

FCDP: fraction of predated phytoplankton carbon produced as dissolved organic carbon

FCD_x: fraction of metabolism excluded as dissolved organic carbon at infinite dissolved oxygen concentration for algal group x

K_{RPOC}: dissolution rate of refractory particulate organic carbon (day⁻¹)

K_{LPOC}: dissolution rate of labile particulate organic carbon (day⁻¹)

K_{HR}: heterotrophic respiration rate of dissolved organic carbon (day⁻¹)

W_{SRP}: settling velocity of refractory particulate organic carbon (m day⁻¹)

W_{SLP}: settling velocity of labile particulate organic carbon (m day⁻¹)

W_{RPOC}: external loads of refractory particulate organic carbon (g[C] day⁻¹)

W_{LPOC}: external loads of labile particulate organic carbon (g[C] day⁻¹)

W_{DOC}: external loads of dissolved organic carbon (g[C] day⁻¹)

K_{HR_x}: half saturation constant of dissolved oxygen for DOC for algal group x (mg [O₂]/L)

Denit: denitrification rate (day⁻¹)

K_{RC}: minimum dissolution rate of refractory particulate organic carbon (day⁻¹)

K_{LC}: minimum dissolution rate of labile particulate organic carbon (day⁻¹)

K_{DC}: minimum respiration rate of dissolved organic carbon (day⁻¹)

K_{RCalg} : constant that relates dissolution of refractory particulate organic carbon to phytoplankton biomass ($\text{day}^{-1} \text{mg}^{-1}[\text{C}] \text{L}$)

K_{LCalg} : constant that relates dissolution of labile particulate organic carbon to phytoplankton biomass ($\text{day}^{-1} \text{mg}^{-1}[\text{C}] \text{L}$)

K_{DCalg} : constant that relates respiration of DOC to phytoplankton biomass ($\text{day}^{-1} \text{mg}^{-1}[\text{C}] \text{L}$)

KT_{HDR} : effect of temperature on hydrolysis of particulate organic matter ($^{\circ}\text{C}$)

KT_{MNL} : effect of temperature on mineralization of dissolved organic matter ($^{\circ}\text{C}$)

TR_{HDR} : reference temperature for hydrolysis of particulate organic matter ($^{\circ}\text{C}$)

TR_{MNL} : reference temperature for mineralization of dissolved organic matter ($^{\circ}\text{C}$)

KH_{ORDO} : oxic respiration half saturation constant for dissolved oxygen ($\text{mg}[\text{O}_2] / \text{L}$)

K_{DOC} : heterotrophic respiration rate of DOC at infinite dissolved oxygen concentration (day^{-1})

KH_{DN} : denitrification half saturation constant for nitrate ($\text{mg}[\text{N}]/\text{L}$)

A_{ANOX} : ratio of denitrification rate to oxic dissolved organic carbon respiration rate

6.1.3 Nitrogen

There are 5 nitrogen species in our model including refractory particulate organic nitrogen (RPON), labile particulate organic nitrogen (LPON), and dissolved organic nitrogen (DON), ammonium nitrogen (NH_4), and nitrite-nitrate nitrogen (NO_3). For particulate organic nitrogen, the source is from the phytoplankton metabolism and predation, while the loss includes hydrolysis and settling of particulate organic nitrogen. For dissolved organic nitrogen, the source includes phytoplankton metabolism, predation and hydrolysis of particulate organic carbon, while the loss is from mineralization. For ammonium nitrogen, the source includes phytoplankton metabolism, phytoplankton predation, mineralization from DON and sediment ammonium flux, while the loss includes phytoplankton uptake and nitrification into nitrate. For nitrate nitrogen, the source includes nitrification from NH_4 and sediment nitrate flux, while the loss includes phytoplankton uptake and denitrification to nitrogen gas.

$$\frac{\partial RPON}{\partial t} = \sum_x (FNR_x \cdot BM_x + FNRP \cdot PR_x) \cdot ANC_x \cdot B_x - K_{RPON} \cdot RPON + \frac{\partial}{\partial z} (WS_{RP} \cdot RPON) + \frac{WRPON}{V} \quad (23)$$

$$\frac{\partial LPON}{\partial t} = \sum_x (FNL_x \cdot BM_x + FNLP \cdot PR_x) \cdot ANC_x \cdot B_x - K_{LPON} \cdot LPON + \frac{\partial}{\partial z} (WS_{LP} \cdot LPON) + \frac{WLPON}{V} \quad (24)$$

$$\frac{\partial DON}{\partial t} = \sum_x (FND_x \cdot BM_x + FNDP \cdot PR_x) ANC_x \cdot B_x + K_{RPON} \cdot RPON + K_{LPON} \cdot LPON - K_{DON} \cdot DON + \frac{WDON}{V} \quad (25)$$

$$\frac{\partial NH4}{\partial t} = \sum_x (FNI_x \cdot BM_x + FNIP \cdot RP_x - PN_x \cdot P_x) ANC_x \cdot B_x + K_{DON} \cdot DON - Nit \cdot NH4 + \frac{BFNH4}{\Delta z} + \frac{WNH4}{V} \quad (26)$$

$$\frac{\partial NO3}{\partial t} = - \sum_x (1 - PN_x) P_x \cdot ANC_x \cdot B_x + Nit \cdot NH4 - ANDC \cdot Denit \cdot DOC + \frac{BFNO3}{\Delta z} + \frac{WNO3}{V} \quad (27)$$

$$PN_x = NH4 \frac{NO3}{(KHN_x + NH4)(KHN_x + NO3)} + NH4 \frac{KHN_x}{(NH4 + NO3)(KHN_x + NO3)} \quad (28)$$

$$K_{RPON} = \left(K_{RN} + \frac{KHN}{KHN + NH4 + NO3} K_{RNA \lg} \sum_x B_x \right) \cdot e^{KT_{HDR} \cdot (T - TR_{HDR})} \quad (29)$$

$$K_{LPON} = \left(K_{LN} + \frac{KHN}{KHN + NH4 + NO3} K_{LNa \lg} \sum_x B_x \right) \cdot e^{KT_{HDR} \cdot (T - TR_{HDR})} \quad (30)$$

$$K_{DON} = \left(K_{DN} + \frac{KHN}{KHN + NH4 + NO3} K_{DNa \lg} \sum_x B_x \right) \cdot e^{KT_{MNL} \cdot (T - TR_{MNL})} \quad (31)$$

$$Nit = \frac{DO}{KHNit_{DO} + DO} \cdot \frac{1}{KHNit_N + NH4} Nit_m \cdot f_{nit}(T) \quad (32)$$

$$f_{nit}(T) = \begin{cases} e^{-KNit1 \cdot (T - TNit)^2}, & \text{if } T \leq TNit \\ e^{-KNit2 \cdot (TNit - T)^2}, & \text{if } T > TNit \end{cases} \quad (33)$$

FNR_x: fraction of metabolized nitrogen by algal group x produced as refractory particulate organic nitrogen

FNL_x: fraction of metabolized nitrogen by algal group x produced as labile particulate organic nitrogen

FND_x : fraction of metabolized nitrogen by algal group x produced as dissolved organic nitrogen
 FNI_x : fraction of metabolized nitrogen by algal group x produced as inorganic nitrogen
 $FNRP$: fraction of predated nitrogen produced as refractory particulate organic nitrogen
 $FNLP$: fraction of predated nitrogen produced as labile particulate organic nitrogen
 $FNDP$: fraction of predated nitrogen produced as dissolved organic nitrogen
 $FNIP$: fraction of predated nitrogen produced as inorganic nitrogen
 ANC_x : nitrogen to carbon ratio for algal group x (g [N] per g[C])
 K_{RPON} : hydrolysis rate of refractory particulate organic nitrogen (day^{-1})
 K_{LPON} : hydrolysis rate of labile particulate organic nitrogen (day^{-1})
 K_{DON} : mineralization rate of dissolved organic nitrogen (day^{-1})
 $WRPON$: external loads of refractory particulate organic nitrogen (g [N]day^{-1})
 $WLPON$: external loads of labile particulate organic nitrogen (g [N]day^{-1})
 $WDON$: external loads of dissolved organic nitrogen (g [N]day^{-1})
 WNH_4 : external loads of ammonium (g [N]day^{-1})
 WNO_3 : external loads of nitrate (g [N]day^{-1})
 PN_x : preference for ammonium uptake by algal group x ($0 \leq PN_x \leq 1$)
 Nit : nitrification rate (day^{-1})
 $BFNH_4$: sediment-water exchange flux of ammonium ($\text{g [N] m}^{-2} \text{day}^{-1}$)
 $BFNO_3$: sediment-water exchange flux of nitrate ($\text{g [N] m}^{-2} \text{day}^{-1}$)
 $ANDC$: mass of nitrate nitrogen reduced per mass of dissolved organic carbon oxidized (g [N] per g[C])
 K_{RN} : minimum hydrolysis rate of refractory particulate organic nitrogen (day^{-1})
 K_{LN} : minimum hydrolysis rate of labile particulate organic nitrogen (day^{-1})
 K_{DN} : minimum mineralization rate of dissolved organic nitrogen (day^{-1})
 K_{RNalg} : constant that relates hydrolysis of RPON to algal biomass (day^{-1} per mg[C]/L)
 K_{LNalg} : constant that relates hydrolysis of LPON to algal biomass (day^{-1} per mg[C]/L)
 K_{DNalg} : constant that relates mineralization of DON to algal biomass (day^{-1} per mg[C]/L)
 KHN : mean half saturation constant for algal nitrogen uptake (mg [N]/L), $KHN = \frac{1}{3} \sum_x KHN_x$
 $KHNit_{DO}$: nitrification half saturation constant for dissolved oxygen ($\text{mg [O}_2\text{]/L}$)
 $KHNit_N$: nitrification half saturation constant for ammonium (mg [N]/L)

Nit_m: maximum nitrification rate at temperature TNit (day⁻¹)

TNit: optimal temperature for nitrification (°C)

KNit1: effect of temperature below TNit for nitrification rate (°C⁻²)

KNit2: effect of temperature above TNit for nitrification rate (°C⁻²)

3.2.4 Phosphorus

There are 4 phosphorus species in our model including refractory particulate organic phosphorus (RPOP), labile particulate organic phosphorus (LPOP), and dissolved organic phosphorus (DOP), and total phosphate (PO₄). For particulate organic phosphorus, the source is from the phytoplankton metabolism and predation, while the loss includes hydrolysis and settling of particulate organic phosphorus. For dissolved organic phosphorus, the source includes phytoplankton metabolism, predation and hydrolysis of particulate organic carbon, while the loss is from mineralization. For total phosphate, the source includes phytoplankton metabolism, phytoplankton predation, mineralization from DOP and sediment phosphate flux, while the loss includes phytoplankton uptake and settling of sorbed phosphate.

$$\frac{\partial RPOP}{\partial t} = \sum_x (FPR_x \cdot BM_x + FPRP \cdot PR_x) \cdot APC \cdot B_x - K_{RPOP} \cdot RPOP + \frac{\partial}{\partial z} (WS_{RP} \cdot RPOP) + \frac{WRPOP}{V} \quad (34)$$

$$\frac{\partial LPOP}{\partial t} = \sum_x (FPL_x \cdot BM_x + FPLP \cdot PR_x) \cdot APC \cdot B_x - K_{LPOP} \cdot LPOP + \frac{\partial}{\partial z} (WS_{LP} \cdot LPOP) + \frac{WLPOP}{V} \quad (35)$$

$$\frac{\partial DOP}{\partial t} = \sum_x (FPD_x \cdot BM_x + FPDp \cdot PR_x) APC \cdot B_x + K_{RPOP} \cdot RPOP + K_{LPOP} \cdot LPOP - K_{DOP} \cdot DOP + \frac{WDOP}{V} \quad (36)$$

$$\frac{\partial PO4_t}{\partial t} = \sum_x (FPI_x \cdot BM_x + FPIP \cdot PR_x - P_x) APC \cdot B_x + K_{DOP} \cdot DOP + \frac{\partial (WS_{TSS} \cdot PO4_p)}{\partial z} + \frac{BFPO4_d}{\Delta z} + \frac{WPO4_t}{V} \quad (37)$$

$$PO4_p = \frac{K_{PO4p} \cdot TSS}{1 + K_{PO4p} \cdot TSS} PO4_t, \quad PO4_d = \frac{1}{1 + K_{PO4p} \cdot TSS} PO4_t \quad (38)$$

$$K_{RPOP} = \left(K_{RP} + \frac{KHP}{KHP + PO4_d} K_{RPa} \sum_x B_x \right) \cdot e^{KT_{HDR} \cdot (T - TR_{HDR})} \quad (39)$$

$$K_{LPOP} = \left(K_{LP} + \frac{KHP}{KHP + PO4_d} K_{LPa} \sum_x B_x \right) \cdot e^{KT_{HDR} \cdot (T - TR_{HDR})} \quad (40)$$

$$K_{DOP} = \left(K_{DP} + \frac{KHP}{KHP + PO4_d} K_{DPa} \sum_x B_x \right) \cdot e^{KT_{MNL} \cdot (T - TR_{MNL})} \quad (41)$$

FPR_x: fraction of metabolized phosphorus by algal group x produced as refractory particulate organic phosphorus

FPL_x: fraction of metabolized phosphorus by algal group x produced as labile particulate organic phosphorus

FPD_x: fraction of metabolized phosphorus by algal group x produced as dissolved organic phosphorus

FPI_x: fraction of metabolized phosphorus by algal group x produced as inorganic phosphorus

FPRP: fraction of predated phosphorus produced as refractory particulate organic phosphorus

FPLP: fraction of predated phosphorus produced as labile particulate organic phosphorus

FPDP: fraction of predated phosphorus produced as dissolved organic phosphorus

FPIP: fraction of predated phosphorus produced as inorganic phosphorus

APC: phosphorus to carbon ratio for algal group x (g [P] per g [C])

K_{RPOP}: hydrolysis rate of refractory particulate organic phosphorus (day⁻¹)

K_{LPOP}: hydrolysis rate of labile particulate organic phosphorus (day⁻¹)

K_{DOP}: mineralization rate of dissolved organic phosphorus (day⁻¹)

WRPOP: external loads of refractory particulate organic phosphorus (g [P]day⁻¹)

WLPOP: external loads of labile particulate organic phosphorus (g [P]day⁻¹)

WDOP: external loads of dissolved organic phosphorus (g [P]day⁻¹)

WPO_{4t}: external loads of total phosphate (g [P]day⁻¹)

WS_{TSS}: settling velocity of suspended solids (m day⁻¹)

PO_{4d}: dissolved phosphate (mg [P]/L)

PO_{4p}: particulate phosphate (mg [P]/L)

$BFPO_{4d}$: sediment-water exchange flux of phosphate (g [P] m⁻² day⁻¹)

K_{RP} : minimum hydrolysis rate of refractory particulate organic phosphorus (day⁻¹)

K_{LP} : minimum hydrolysis rate of labile particulate organic phosphorus (day⁻¹)

K_{DP} : minimum mineralization rate of dissolved organic phosphorus (day⁻¹)

K_{RPalg} : constant that relates hydrolysis of RPOP to algal biomass (day⁻¹ per mg P/L)

K_{LPalg} : constant that relates hydrolysis of LPOP to algal biomass (day⁻¹ per mg [P]/L)

K_{DPalg} : constant that relates mineralization of DOP to algal biomass (day⁻¹ per mg [P]/L)

KHP : mean half saturation constant for algal phosphorus uptake (mg [P]/L), $KHP = \frac{1}{3} \sum_x KHP_x$

K_{PO_4p} : empirical coefficient relating phosphate sorption to total suspended solid (per mg/L)

3.2.5 Silica

There are 2 silica species in our model including particulate biogenic silica (SU) and available silica (SA). For particulate biogenic silica, the source is from the phytoplankton metabolism and predation, while the loss includes dissolution and settling of particulate biogenic silica. For available silica, the source is from the phytoplankton metabolism, predation, dissolution of particulate biogenic silica and sediment available silica flux, while the loss includes phytoplankton uptake and settling of particulate biogenic silica.

$$\frac{\partial SU}{\partial t} = (FSP_d \cdot BM_d + FSPP \cdot PR_d) ASC_d \cdot B_d - K_{SUA} \cdot SU + \frac{\partial (WS_d \cdot SU)}{\partial z} + \frac{WSU}{V} \quad (42)$$

$$\frac{\partial SA}{\partial t} = (FSI_d \cdot BM_d + FSIP \cdot PR_d - P_d) ASC_d \cdot B_d + K_{SUA} \cdot SU + \frac{\partial (WS_{TSS} \cdot SA_p)}{\partial z} + \frac{BFSA_d}{\Delta z} + \frac{WSA}{V} \quad (43)$$

$$SA_p = \frac{K_{SAp} \cdot TSS}{1 + K_{SAp} \cdot TSS} SA_t, \quad SA_d = \frac{1}{1 + K_{SAp} \cdot TSS} SA_t \quad (44)$$

$$K_{SUA} = K_{SU} \cdot e^{KT_{SUA}(T - TR_{SUA})} \quad (45)$$

FSP_d : fraction of metabolized silica by diatom produced as particulate biogenic silica

FSI_d : fraction of metabolized silica by diatom produced as available silica

FSPP: fraction of predated diatom silica produced as particulate biogenic silica
 FSIP: fraction of predated diatom silica produced as available silica
 ASC_d: silica to carbon ratio for diatom (g [Si] per g[C])
 K_{SUA}: dissolution rate of particulate biogenic silica (day⁻¹)
 WSU: external loads of particulate biogenic silica (g [Si] day⁻¹)
 WSA: external loads of available silica (g [Si] day⁻¹)
 SA_d: dissolved available silica (mg [Si]/L)
 SA_p: sorbed available silica (mg [Si]/L)
 BFSAD: sediment-water exchange flux of available silica (g [Si] m⁻² day⁻¹)
 K_{SAP}: empirical coefficient relating available silica sorption to total suspended solid (per mg/L)
 K_{SU}: dissolution rate of particulate biogenic silica at TR_{SUA} (day⁻¹)
 KT_{SUA}: effect of temperature on dissolution of particulate biogenic silica (°C⁻¹)
 TR_{SUA}: reference temperature for dissolution of particulate biogenic silica (°C)

3.2.6 Chemical Oxygen Demand

In the model, there is chemical oxygen demand that represents the reduced substances. The source is from chemical oxygen demand from sediment, while the loss is through oxidization.

$$\frac{\partial COD}{\partial t} = -\frac{DO}{KH_{COD} + DO} K_{COD} \cdot COD + \frac{BFCOD}{\Delta z} + \frac{WCOD}{V} \quad (46)$$

$$K_{COD} = K_{CD} \cdot e^{KT_{COD}(T-TR_{COD})} \quad (47)$$

KH_{COD}: half saturation constant of dissolved oxygen required for oxidation of chemical oxygen demand (mg[O₂]/L)
 K_{COD}: oxidation rate of chemical oxygen demand (day⁻¹)
 BFCOD: sediment-water exchange flux of chemical oxygen demand (g [O₂] m⁻² day⁻¹)
 WCOD: external loads of chemical oxygen demand (g [O₂] day⁻¹)
 K_{CD}: oxidation rate of chemical oxygen demand at TR_{COD} (day⁻¹)
 KT_{COD}: effect of temperature on oxidation of chemical oxygen demand (°C⁻¹)
 TR_{COD}: reference temperature for oxidation of chemical oxygen demand (°C)

3.2.7 Dissolved Oxygen

There are one dissolved oxygen (DO) species in our model. The source includes photosynthesis and surface reaeration, while the loss includes phytoplankton metabolism, nitrification, heterotrophic respiration, oxidation of chemical oxygen demand, and sediment oxygen demand.

$$\frac{\partial DO}{\partial t} = \sum_x \left[(1.3 - 0.3 \cdot PN_x) P_x - (1 - FCD_x) \frac{DO}{K_{HR_x} + DO} BM_x \right] AOCR \cdot B_x - AONT \cdot Nit \cdot NH_4 \quad (48)$$

$$- AOCR \cdot K_{HR} \cdot DOC - \frac{DO}{K_{H_{COD}} + DO} KCOD \cdot COD + K_r (DO_s - DO) + \frac{SOD}{\Delta z} + \frac{WDO}{V} \quad)$$

$$K_r = Area \cdot Rv \cdot WMS^{1.5} \quad (49)$$

$$Rv = 0.54 + 0.0233 \cdot T - 0.0020 \cdot S \quad (50)$$

$$DO_s = 14.6244 - 0.367134 \cdot T + 4.497 \times 10^{-3} \cdot T^2 - (9.66 \times 10^{-2} - 2.05 \times 10^{-3} \cdot T - 2.739 \times 10^{-4} \cdot S) \cdot S \quad (51)$$

AOCR: dissolved oxygen to carbon ratio in respiration (g [O₂] per g [C])

AONT: mass of dissolved oxygen consumed per unit mass of ammonium nitrogen nitrified (g [O₂] per g[N])

K_r: reaeration coefficient (day⁻¹)

DO_s: saturated concentration of dissolved oxygen (mg [O₂]/L)

SOD: sediment oxygen demand (g [O₂] m⁻² day⁻¹)

WDO: external loads of dissolved oxygen (g [O₂] day⁻¹)

Area: empirical constant

Rv: ratio of kinematic viscosity of pure water at 20 °C to kinematic viscosity of water at specified temperature and salinity

WMS: wind speed measured at 10 m above water surface (m/s)

6.2 ICM 21

When zooplankton kinetics are added in the model, the model becomes more complex. Not only zooplankton will graze on phytoplankton, but also it can graze on organic carbon species. Furthermore, the metabolism and death of zooplankton provides sources to carbon and nutrient pools. In this section, I will try to use the same variable names in the parameter file `icm.in`. If the variable names are not mentioned specifically here, they should be explained already in section 4 Model Parameters. More details about the zooplankton dynamics can be found in (Wang and Kuo, 2009)

6.2.1 Zooplankton

There are two zooplankton species. The only source of zooplankton is growth by predation on other species, while the sink of zooplankton includes basal metabolism and mortality. Here, the mortality of zooplankton includes death and predation by higher trophic levels and the other zooplankton species. Below are the equations related to zooplankton dynamics in the ICM model.

$$\frac{\partial ZB_j}{\partial t} = (GZ_j - BMZ_j - PRZ_j) \cdot ZB_j \quad (52)$$

$$GZ_j = \sum_{i=1}^8 S_{ij} \cdot Eff \cdot (1 - RF) \cdot f_j(T) \quad (53)$$

$$BMZ_j = BMZR_j \cdot e^{rKBZ_j \cdot (T - TBZ_j)} \quad (54)$$

$$PRZ_j \cdot ZB_j = \left[\frac{GZM_{ij} \cdot \frac{PPC_{ij}}{rKhGE_{ij}} \cdot ZB_i}{1 + \sum_{m=1}^8 \frac{PPC_{mj}}{rKhGE_{mj}} \cdot nz_m} \right] \cdot ZB_j \cdot f_j(T), i \neq j \quad (55)$$

$$+ \left[RZ_j \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) + DRZ_j \right] \cdot ZB_j$$

$$S_{ij} = \frac{GZM_{ij} \cdot \frac{PPC_{ij}}{rKhGE_{ij}} \cdot nz_i}{1 + \sum_{m=1}^8 \frac{PPC_{mj}}{rKhGE_{mj}} \cdot nz_m} \quad (56)$$

$$f_j(T) = \begin{cases} e^{-rKTGZ1_j \cdot (T-TGZ_j)^2}, & \text{if } T > TGZ_j \\ e^{-rKTGZ2_j \cdot (TGZ_j-T)^2}, & \text{if } T \leq TGZ_j \end{cases} \quad (57)$$

GZ_j : growth rate of zooplankton j (day⁻¹)

BMZ_j : basal metabolism rate of zooplankton j (day⁻¹)

PRZ_j : mortality rate of zooplankton j (day⁻¹)

nz_i : represent the prey of zooplankton including ZB_j , PB_i , RPOC, LPOC and DOC. The numbering of the index is shown in the table below.

Table 3

nz_i	ZB1	ZB2	PB1	PB2	PB3	RPOC	LPOC	DOC
index	1	2	3	4	5	6	7	8

6.2.2 Phytoplankton

For phytoplankton, only the predation term is modified when zooplankton dynamics are added. Therefore, the equations in section 6.1.1 Phytoplankton keep the same. Only the term $PR_x \cdot PB_x$ in Equation (9) are replaced by

$$PR_x \cdot PB_x = PR_i \cdot PB_i = \sum_{j=1}^2 S_{ij} \cdot ZB_j \cdot f_j(T) + Pf \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) \cdot PB_i \quad (58)$$

The first term on the RHS is phytoplankton predated by zooplankton, while the second term is phytoplankton predated by higher trophic level.

6.2.3 Carbon

Compared to the equations in section 6.1.2 Carbon, there are many changes after zooplankton dynamics are added in the model. Below are the equations for RPOC, LPOC and DOC. On the RHS and each equation, there is an annotation for the additional terms which are related to

zooplankton or higher trophic level predation. For example, ZB->PB means that this term accounts for the phytoplankton grazed by zooplankton. Except from these addition terms, the other terms keep the same as ICM 19 model.

$$\begin{aligned}
\frac{\partial RPOC}{\partial t} = & - \sum_{\substack{j=1 \\ i=6}}^2 S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [RF + Eff \cdot (1 - RF)], & \text{ZB} \rightarrow \text{RPOC} \\
& + FCRPZ \cdot \sum_{j=1}^2 \sum_{\substack{i=1 \\ i \neq j}}^2 S_{ij} \cdot ZB_j \cdot f_j(T) \cdot (1 - RF) \cdot (1 - Eff), & \text{ZB} \rightarrow \text{ZB} \\
& + FCRPZ \cdot \sum_{j=1}^2 \left[RZ_j \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) + DRZ_j \right] \cdot ZB_j, \text{Fish} \rightarrow \text{ZB \& ZB death} & (59) \\
& + FCRP \cdot \sum_{j=1}^2 \sum_{i=3}^5 S_{ij} \cdot ZB_j \cdot f_j(T) \cdot (1 - RF) \cdot (1 - E), & \text{ZB} \rightarrow \text{PB} \\
& + FCRP \cdot \sum_{i=3}^5 Pf \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) \cdot PB_i, & \text{Fish} \rightarrow \text{PB} \\
& - K_{RPOC} \cdot RPOC + \frac{\partial}{\partial Z} (WS_{RP} \cdot RPOC) + \frac{WRPOC}{V}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial LPOC}{\partial t} = & - \sum_{\substack{j=1 \\ i=7}}^2 S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [RF + Eff \cdot (1 - RF)], & \text{ZB} \rightarrow \text{LPOC} \\
& + FCLPZ \cdot \sum_{j=1}^2 \sum_{\substack{i=1 \\ i \neq j}}^2 S_{ij} \cdot ZB_j \cdot f_j(T) \cdot (1 - RF) \cdot (1 - Eff), & \text{ZB} \rightarrow \text{ZB} \\
& + FCLPZ \cdot \sum_{j=1}^2 \left[RZ_j \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) + DRZ_j \right] \cdot ZB_j, \text{Fish} \rightarrow \text{ZB \& ZB death} & (60) \\
& + FCLP \cdot \sum_{j=1}^2 \sum_{i=3}^5 S_{ij} \cdot ZB_j \cdot f_j(T) \cdot (1 - RF) \cdot (1 - E), & \text{ZB} \rightarrow \text{PB} \\
& + FCLP \cdot \sum_{i=3}^5 Pf \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) \cdot PB_i, & \text{Fish} \rightarrow \text{PB} \\
& - K_{LPOC} \cdot LPOC + \frac{\partial}{\partial Z} (WS_{LP} \cdot LPOC) + \frac{WLPOC}{V}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial DOC}{\partial t} = & -\sum_{\substack{j=1 \\ i=8}}^2 S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [RF + Eff \cdot (1 - RF)], & ZB \rightarrow DOC \\
& + FCDPZ \cdot \sum_{j=1}^2 \sum_{\substack{i=1 \\ i \neq j}}^2 S_{ij} \cdot ZB_j \cdot f_j(T) \cdot (1 - RF) \cdot (1 - Eff), & ZB \rightarrow ZB \\
& + FCDPZ \cdot \sum_{j=1}^2 \left[RZ_j \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) + DRZ_j \right] \cdot ZB_j, & \text{Fish} \rightarrow ZB \text{ \& } ZB \text{ death} \\
& + FCDP \cdot \sum_{j=1}^2 \sum_{i=3}^5 S_{ij} \cdot ZB_j \cdot f_j(T) \cdot (1 - RF) \cdot (1 - E), & ZB \rightarrow PB \\
& + FCDP \cdot \sum_{i=3}^5 Pf \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) \cdot PB_i, & \text{Fish} \rightarrow PB \\
& + \sum_{j=1}^2 \left[FCDZ_j + (1 - FCDZ_j) \frac{KHRZ_j}{KHRZ_j + DO} \right] BMZ_j \cdot ZB_j & ZB \text{ metabolism} \\
& + \sum_{i=1}^3 \left[FCD_i + (1 - FCD_i) \frac{KHR_i}{KHR_i + DO} \right] BMP_i \cdot PB_i & PB \text{ metabolism} \\
& + K_{RPOC} \cdot RPOC + K_{LPOC} \cdot LPOC - K_{HR} \cdot DOC - Denit \cdot DOC + \frac{WDOC}{V}
\end{aligned} \tag{61}$$

Note the symbol BM_x in Equation (1) is replaced by the symbol BMP_i in Equation (61)

6.2.4 Nitrogen

Below are the equations for RPON, LPON, DON and NH4. The equation for NO3 in ICM 21 keeps the same as in ICM 19.

$$\begin{aligned}
\frac{\partial RPON}{\partial t} = & FNRPZ \cdot \sum_{j=1}^2 \sum_{\substack{i=1 \\ i \neq j}}^2 ANCZ_j \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], \quad ZB \rightarrow ZB \\
& + FNRPZ \cdot \sum_{j=1}^2 \left[RZ_j \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) + DRZ_j \right] \cdot ZB_j \cdot ANCZ_j, \quad \begin{cases} \text{Fish} \rightarrow ZB \\ \text{ZB death} \end{cases} \\
& + FNRP \cdot \sum_{j=1}^2 \sum_{i=3}^5 ANC_i \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], \quad ZB \rightarrow PB \\
& + FNRP \cdot \sum_{i=3}^5 ANC_i \cdot Pf \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) \cdot PB_i, \quad \text{Fish} \rightarrow PB \quad (62) \\
& + \sum_{j=1}^2 FNRZ_j \cdot BMZ_j \cdot ZB_j \cdot ANCZ_j \quad \text{ZB metabolism} \\
& + \sum_{i=1}^3 FNR_i \cdot BMP_i \cdot ANC_i \cdot PB_i \quad \text{PB metabolism} \\
& - K_{RPOC} \cdot RPOC + \frac{\partial}{\partial z} (WS_{LP} \cdot RPON) + \frac{WRPON}{V}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial LPON}{\partial t} = & FNLpz \cdot \sum_{j=1}^2 \sum_{\substack{i=1 \\ i \neq j}}^2 ANCZ_j \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], \quad ZB \rightarrow ZB \\
& + FNLpz \cdot \sum_{j=1}^2 \left[RZ_j \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) + DRZ_j \right] \cdot ZB_j \cdot ANCZ_j, \quad \begin{cases} \text{Fish} \rightarrow ZB \\ \text{ZB death} \end{cases} \\
& + FNLp \cdot \sum_{j=1}^2 \sum_{i=3}^5 ANC_i \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], \quad ZB \rightarrow PB \\
& + FNLp \cdot \sum_{i=3}^5 ANC_i \cdot Pf \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) \cdot PB_i, \quad \text{Fish} \rightarrow PB \quad (63) \\
& + \sum_{j=1}^2 FNLz_j \cdot BMZ_j \cdot ZB_j \cdot ANCZ_j \quad \text{ZB metabolism} \\
& + \sum_{i=1}^3 FNL_i \cdot BMP_i \cdot ANC_i \cdot PB_i \quad \text{PB metabolism} \\
& - K_{LPoc} \cdot LPON + \frac{\partial}{\partial z} (WS_{LP} \cdot LPON) + \frac{WLPON}{V}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial DON}{\partial t} = & FNDPZ \cdot \sum_{j=1}^2 \sum_{\substack{i=1 \\ i \neq j}}^2 ANCZ_j \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], & ZB \rightarrow ZB \\
& + FNDPZ \cdot \sum_{j=1}^2 \left[RZ_j \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) + DRZ_j \right] \cdot ZB_j \cdot ANCZ_j, & \begin{cases} \text{Fish} \rightarrow ZB \\ \text{ZB death} \end{cases} \\
& + FNDP \cdot \sum_{j=1}^2 \sum_{i=3}^5 ANC_i \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], & ZB \rightarrow PB \\
& + FNDP \cdot \sum_{i=3}^5 ANC_i \cdot Pf \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) \cdot PB_i, & \text{Fish} \rightarrow PB \quad (64) \\
& + \sum_{j=1}^2 FNDZ_j \cdot BMZ_j \cdot ZB_j \cdot ANCZ_j & \text{ZB metabolism} \\
& + \sum_{i=1}^3 FND_i \cdot BMP_i \cdot ANC_i \cdot PB_i & \text{PB metabolism} \\
& + K_{RPON} \cdot RPON + K_{LPON} \cdot LPON - K_{DON} \cdot DON + \frac{WDON}{V}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial NH4}{\partial t} = & FNIPZ \cdot \sum_{j=1}^2 \sum_{\substack{i=1 \\ i \neq j}}^2 ANCZ_j \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], & ZB \rightarrow ZB \\
& + FNIPZ \cdot \sum_{j=1}^2 \left[RZ_j \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) + DRZ_j \right] \cdot ZB_j \cdot ANCZ_j, & \begin{cases} \text{Fish} \rightarrow ZB \\ \text{ZB death} \end{cases} \\
& + FNIP \cdot \sum_{j=1}^2 \sum_{i=3}^5 ANC_i \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], & ZB \rightarrow PB \\
& + FNIP \cdot \sum_{i=3}^5 ANC_i \cdot Pf \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) \cdot PB_i, & \text{Fish} \rightarrow PB \quad (65) \\
& + \sum_{j=1}^2 FNIZ_j \cdot BMZ_j \cdot ZB_j \cdot ANCZ_j & \text{ZB metabolism} \\
& + \sum_{i=1}^3 FNI_i \cdot BMP_i \cdot ANC_i \cdot PB_i & \text{PB metabolism} \\
& - \sum_{i=1}^3 PN_i \cdot P_i \cdot APC_i \cdot PB_i + K_{DON} \cdot DON - Nit \cdot NH4 + \frac{BFNH4}{\Delta z} + \frac{WNH4}{V}
\end{aligned}$$

Note, please refer to ICM 19 for the meanings of PN_i and P_i

6.2.5 Phosphorus

Below are the equations for RPOP, LPOP, DOP and PO4t.

$$\begin{aligned}
\frac{\partial RPOP}{\partial t} = & FPRPZ \cdot \sum_{j=1}^2 \sum_{\substack{i=1 \\ i \neq j}}^2 APCZ_j \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], & ZB \rightarrow ZB \\
& + FPRPZ \cdot \sum_{j=1}^2 \left[RZ_j \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) + DRZ_j \right] \cdot ZB_j \cdot APCZ_j, & \begin{cases} \text{Fish} \rightarrow ZB \\ \text{ZB death} \end{cases} \\
& + FPRP \cdot \sum_{j=1}^2 \sum_{i=3}^5 APC_i \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], & ZB \rightarrow PB \\
& + FPRP \cdot \sum_{i=3}^5 APC_i \cdot Pf \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) \cdot PB_i, & \text{Fish} \rightarrow PB \quad (66) \\
& + \sum_{j=1}^2 FPRZ_j \cdot BMZ_j \cdot ZB_j \cdot APCZ_j & \text{ZB metabolism} \\
& + \sum_{i=1}^3 FPR_i \cdot BMP_i \cdot APC_i \cdot PB_i & \text{PB metabolism} \\
& - K_{RPOP} \cdot RPOP + \frac{\partial}{\partial Z} (WS_{RP} \cdot RPOP) + \frac{WRPOP}{V}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial LPOP}{\partial t} = & FPLPZ \cdot \sum_{j=1}^2 \sum_{\substack{i=1 \\ i \neq j}}^2 APCZ_j \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], & ZB \rightarrow ZB \\
& + FPLPZ \cdot \sum_{j=1}^2 \left[RZ_j \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) + DRZ_j \right] \cdot ZB_j \cdot APCZ_j, & \begin{cases} \text{Fish} \rightarrow ZB \\ \text{ZB death} \end{cases} \\
& + FPLP \cdot \sum_{j=1}^2 \sum_{i=3}^5 APC_i \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], & ZB \rightarrow PB \\
& + FPLP \cdot \sum_{i=3}^5 APC_i \cdot Pf \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) \cdot PB_i, & \text{Fish} \rightarrow PB \quad (67) \\
& + \sum_{j=1}^2 FPLZ_j \cdot BMZ_j \cdot ZB_j \cdot APCZ_j & \text{ZB metabolism} \\
& + \sum_{i=1}^3 FPL_i \cdot BMP_i \cdot APC_i \cdot PB_i & \text{PB metabolism} \\
& - K_{LPOP} \cdot LPOP + \frac{\partial}{\partial Z} (WS_{LP} \cdot LPOP) + \frac{WLPOP}{V}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial DOP}{\partial t} = & FPDPZ \cdot \sum_{j=1}^2 \sum_{\substack{i=1 \\ i \neq j}}^2 APCZ_j \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], \quad ZB \rightarrow ZB \\
& + FPDPZ \cdot \sum_{j=1}^2 \left[RZ_j \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) + DRZ_j \right] \cdot ZB_j \cdot APCZ_j, \quad \begin{cases} \text{Fish} \rightarrow ZB \\ \text{ZB death} \end{cases} \\
& + FPDP \cdot \sum_{j=1}^2 \sum_{i=3}^5 APC_i \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], \quad ZB \rightarrow PB \\
& + FPDP \cdot \sum_{i=3}^5 APC_i \cdot Pf \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) \cdot PB_i, \quad \text{Fish} \rightarrow PB \quad (68) \\
& + \sum_{j=1}^2 FPDZ_j \cdot BMZ_j \cdot ZB_j \cdot APCZ_j \quad \text{ZB metabolism} \\
& + \sum_{i=1}^3 FPD_i \cdot BMP_i \cdot APC_i \cdot PB_i \quad \text{PB metabolism} \\
& + K_{RPOP} \cdot RPOP + K_{LPOP} \cdot LPOP - K_{DOP} \cdot DOP + \frac{WDOP}{V}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial PO4_t}{\partial t} = & FPIPZ \cdot \sum_{j=1}^2 \sum_{\substack{i=1 \\ i \neq j}}^2 APCZ_j \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], \quad ZB \rightarrow ZB \\
& + FPIPZ \cdot \sum_{j=1}^2 \left[RZ_j \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) + DRZ_j \right] \cdot ZB_j \cdot APCZ_j, \quad \begin{cases} \text{Fish} \rightarrow ZB \\ \text{ZB death} \end{cases} \\
& + FPIP \cdot \sum_{j=1}^2 \sum_{i=3}^5 APC_i \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], \quad ZB \rightarrow PB \\
& + FPIP \cdot \sum_{i=3}^5 APC_i \cdot Pf \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) \cdot PB_i, \quad \text{Fish} \rightarrow PB \quad (69) \\
& + \sum_{j=1}^2 FPIZ_j \cdot BMZ_j \cdot ZB_j \cdot APCZ_j \quad \text{ZB metabolism} \\
& + \sum_{i=1}^3 FPI_i \cdot BMP_i \cdot APC_i \cdot PB_i \quad \text{PB metabolism} \\
& - \sum_{i=1}^3 P_i \cdot APC_i \cdot PB_i + K_{DOP} \cdot DOP + \frac{\partial (WS_{TSS} \cdot PO4_p)}{\partial z} + \frac{BFPO4_d}{\Delta z} + \frac{WPO4_t}{V}
\end{aligned}$$

6.2.6 Silica

Below are the equations for RPOP, LPOP, DOP and PO4t.

$$\begin{aligned}
\frac{\partial SU}{\partial t} = & FSPPZ \cdot \sum_{j=1}^2 \sum_{\substack{i=1 \\ i \neq j}}^2 ASCZ_j \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], \quad ZB \rightarrow ZB \\
& + FSPPZ \cdot \sum_{j=1}^2 \left[RZ_j \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) + DRZ_j \right] \cdot ZB_j \cdot ASCZ_j, \begin{cases} \text{Fish} \rightarrow ZB \\ \text{ZB death} \end{cases} \\
& + FSPP \cdot \sum_{\substack{j=1 \\ i=3}}^2 ASC_d \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], \quad ZB \rightarrow \text{diatom} \\
& + FSPP \cdot ASC_d \cdot Pf \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) \cdot PB_1, \quad \text{Fish} \rightarrow \text{diatom} \\
& + \sum_{j=1}^2 FSPZ_j \cdot BMZ_j \cdot ZB_j \cdot ASCZ_j \quad \text{ZB metabolism} \\
& + FSP_d \cdot BMP_d \cdot ASC_d \cdot PB_1 \quad \text{Diatom metabolism} \\
& - K_{SUA} \cdot SU + \frac{\partial(W S_d \cdot SU)}{\partial z} + \frac{WSU}{V}
\end{aligned} \tag{70}$$

$$\begin{aligned}
\frac{\partial SA}{\partial t} = & FSIPZ \cdot \sum_{j=1}^2 \sum_{\substack{i=1 \\ i \neq j}}^2 ASCZ_j \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], \quad ZB \rightarrow ZB \\
& + FSIPZ \cdot \sum_{j=1}^2 \left[RZ_j \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) + DRZ_j \right] \cdot ZB_j \cdot ASCZ_j, \begin{cases} \text{Fish} \rightarrow ZB \\ \text{ZB death} \end{cases} \\
& + FSIP \cdot \sum_{\substack{j=1 \\ i=3}}^2 ASC_d \cdot S_{ij} \cdot ZB_j \cdot f_j(T) \cdot [1 - Eff \cdot (1 - RF)], \quad ZB \rightarrow \text{diatom} \\
& + FSIP \cdot ASC_d \cdot Pf \cdot \left(\sum_{m=1}^2 ZB_m + \sum_{m=1}^3 PB_m \right) \cdot PB_1, \quad \text{Fish} \rightarrow \text{diatom} \\
& + \sum_{j=1}^2 FSIZ_j \cdot BMZ_j \cdot ZB_j \cdot ASCZ_j \quad \text{ZB metabolism} \\
& + FSI_d \cdot BMP_d \cdot ASC_d \cdot PB_1 \quad \text{diatom metabolism} \\
& - P_d \cdot ASC_d \cdot PB_1 + K_{SUA} \cdot SU + \frac{\partial(W S_{TSS} \cdot SA_p)}{\partial z} + \frac{BFSA_d}{\Delta z} + \frac{WSA}{V}
\end{aligned} \tag{71}$$

6.2.7 Dissolved oxygen

The equation for COD in ICM 21 is the same as in ICM 19. For DO, there is an additional term from zooplankton metabolism and the new equation is

$$\begin{aligned}
\frac{\partial DO}{\partial t} = & \sum_{j=1}^2 (1 - FCDZ_j) \cdot \frac{DO}{KHRZ_j + DO} \cdot BMZ_j \cdot AOCR \cdot ZB_j \\
& + \sum_{i=1}^3 \left[(1.3 - 0.3 \cdot PN_i) P_i - (1 - FCD_i) \frac{DO}{KHR_i + DO} BM_i \right] \cdot AOCR \cdot PB_i \\
& - AONT \cdot Nit \cdot NH4 - AOCR \cdot K_{HR} \cdot DOC - \frac{DO}{KH_{COD} + DO} KCOD \cdot COD \\
& + K_r (DO_s - DO) + \frac{SOD}{\Delta z} + \frac{WDO}{V}
\end{aligned} \tag{72}$$

6.3 Sediment Flux Model

One significant component of our water quality model is the coupling of the water column process with a sediment flux sub-model. The sediment flux model is based on principle of mass conservation. It is consisted of three primary features. First, there are three fluxes: the depositional fluxes of particulate matters from the water column to the benthic bed, the diagenesis flues from the decay of particulate matter in the bed and the sediment fluxes of dissolved nutrient from the bed back into the overlying water. Second, there is a two-layer structure of the benthic bed: a thin aerobic/anaerobic upper layer and a permanently anaerobic lower layer. Third, particulate organic matters are presented in three G classes in the benthic sediments: they are split into three fractions (G classes) based on their decay rates. The details can found in (DiToro and Fitzpatrick 1993).

6.3.1 General introduction

Figure 3 shows the general structures of sediment flux model in the ICM model. It gives out the procedure how sediment fluxes are calculated.

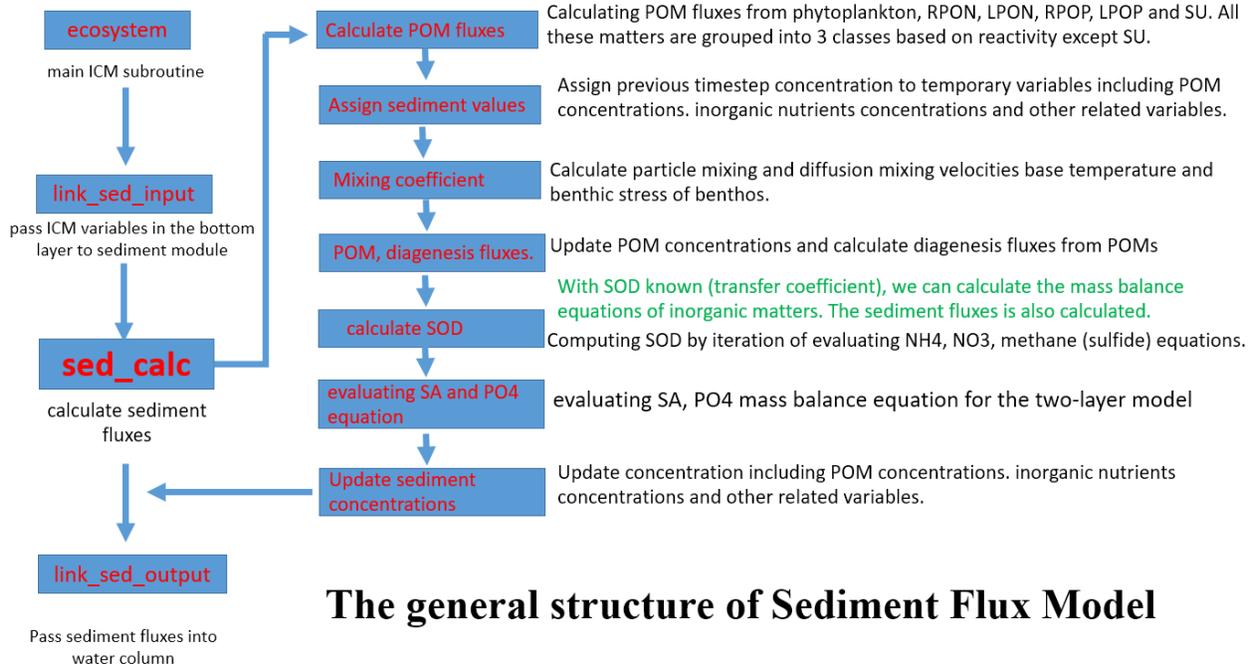


Figure 3. the general structures of sediment flux model in ICM

6.3.2 mass-balance equation

The sediment flux model is based on the assumption of two layers: upper layer (thin) and lower layer (thick). The sediment fluxes is based on the concentration difference between upper layer and bottom layer in the water column. Between the two layers in the sediment, there are also exchanges for all nutrients due to diffusive mixing and particle mixing. Besides, there are reactions that one nutrients specie can be transformed into another. Furthermore, nutrients can be lost by burial in the lower layers. The mass balance equations for the upper and lower layers are:

$$s \cdot (fd_0 \cdot Ct_0 - fd_1 \cdot Ct_1) + KL \cdot (fd_2 \cdot Ct_2 - fd_1 \cdot Ct_1) + \varpi \cdot (fp_2 \cdot Ct_2 - fp_1 \cdot Ct_1) - \frac{k_1^2}{s} Ct_1 + J_1 = 0 \quad (73)$$

$$H_2 \frac{\partial Ct_2}{\partial t} = -KL \cdot (fd_2 \cdot Ct_2 - fd_1 \cdot Ct_1) - \varpi \cdot (fp_2 \cdot Ct_2 - fp_1 \cdot Ct_1) + W \cdot (Ct_1 - Ct_2) - k_2 \cdot Ct_2 + J_2 \quad (74)$$

In these two equations, subscript “0” represents water column; subscript “1” represents the upper sediment layer; and subscript “2” represents the bottom sediment layer. fp_i is the particulate fraction of total substance concentration Ct_i , while fd_i is the dissolved fraction.

$$s = \frac{SOD}{DO_0} : \text{surface transfer coefficient (m/day)}$$

KL: diffusion velocity for dissolved substance between upper and lower layers (m/day)

ϖ : particle mixing velocity between upper and lower layers (m/day).

W: burial rate (m/day)

k_1 and k_2 : reaction velocities in upper and lower layers respectively (m/day). These two terms are calculated based on formulation related to temperature and other factors.

j_1 and j_2 : summation of internal sources in upper and lower layers respectively (m/day). These source include diagenesis fluxes which are from the remineralization of POM in the sediment. In the model, the reaction coefficients of POM related to temperature are normally specified. In the upper layer, there is no diagenesis fluxes because it is very thin and the diagenesis flux is negligible. j_1 is zero for all nutrients in the upper layer except for NO₃ which has source from nitrification of NH₄.

Overall, the equations (73) and (74) can be solved as below after discretization:

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} * \begin{bmatrix} Ct_1^{n+1} \\ Ct_2^{n+1} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \quad (75)$$

Where superscript “n+1” represent the value at the next time step and

$$a_{11} = (KL \cdot fd_1 + \varpi \cdot fp_1 + W) + s \cdot fd_1 + \frac{k_1^2}{s}$$

$$a_{12} = -(KL \cdot fd_2 + \varpi \cdot fp_2)$$

$$a_{21} = -(KL \cdot fd_1 + \varpi \cdot fp_1 + W)$$

$$a_{22} = (KL \cdot fd_2 + \varpi \cdot fp_2) + W + k_2 + H_2 / dt, \quad dt \text{ is time step}$$

$$b_1 = j_1^{n+1} + s \cdot fd_0 \cdot Ct_0^{n+1}$$

$$b_2 = j_2^{n+1} + Ct_2 \frac{H_2}{dt}$$

For a certain substance, when all the items in Equation (75) are specified, we can get the concentrations of Ct_1^{n+1} and Ct_2^{n+1} . In the ICM code, this is done in the subroutine `sed_eq`.

6.4 pH Model

pH model is based on aquatic chemical equilibrium. In the water column, there are many acids/bases among which many processes happen. Some processes are due to the chemical reactions or transformations of chemical substances, while some other processes are related to biological activities. These processes affect the pH variations. The pH model aims to simulate these processes and we further incorporated this model into our water quality model. In the pH model, there are four state variables: total inorganic carbon (TIC), alkalinity (ALK), dissolved calcium ion Ca^{2+} (CA), and solid-phase calcium carbonate ($CaCO_3$). Besides TIC and ALK, calcium species are introduced into our model because calcium usually has high concentration in common found water systems and can impact the PH system. Calcium plays an important role in many biogeochemical processes. In addition, calcium species comprise a buffer system. For instance, acid water with too much aqueous CO_2 will dissolve calcium carbonate and the acidity of the water will be reduced (pH will increase). The reverse reaction will form calcium carbonate and will cause CO_2 lost from the water (pH will decrease).

For TIC, the source terms include oxic respiration of phytoplankton, heterotrophic respiration of DOC, oxidation of organic matter in the sediment, while the loss term is phytoplankton uptake in photosynthesis. Also, the gas exchange between water and air can alter the CO_2 concentration in the water. Moreover, the formation/dissolution of calcium carbonate can decrease/increase CO_2 concentration. For alkalinity, we will consider the effect of NH_4 and NO_3 uptake by phytoplankton. (Ref) mentioned that alkalinity will decrease 15/14 mole when 1 mole of NH_4 is utilized, and will increase 17/16 mole when 1 mole of NO_3 is utilized. Plus, nitrification and the formation/dissolution of calcium carbonate can change alkalinity concentration. The only processes that influence CA concentration is the formation/dissolution of calcium carbonate. The $CaCO_3$ concentration can be altered by the formation/dissolution of calcium carbonate as well as its settling. The following are the mass balance equations for these four variables.

$$\begin{aligned} \frac{\partial TIC}{\partial t} = \sum_x \left\{ (1 - FCD_x) \frac{DO}{K_{HR_x} + DO} BM_x - P_x \right\} B_x + \frac{rKa \cdot (CO2_{sat} - CO2)}{\Delta z} + K_{HR} \cdot DOC \\ + \frac{SOD}{\Delta z \cdot AOC} + rKCAC03 \cdot (CA_{sat} - CA) \frac{mC}{mCAC03} \end{aligned} \quad (76)$$

$$\frac{\partial ALK}{\partial t} = \sum_x \left[-\frac{15}{14} PN_x P_x B_x + \frac{17}{16} (1 - PN_x) P_x B_x \right] ANC_x \frac{mCACO3}{2 \cdot mN} - Nit \cdot NH4 \cdot \frac{mCACO3}{mN} + rKCACO3 \cdot (CA_{sat} - CA) \quad (77)$$

$$\frac{\partial CA}{\partial t} = rKCACO3 \cdot (CA_{sat} - CA) \quad (78)$$

$$\frac{\partial CACO3}{\partial t} = -rKCACO3 \cdot (CA_{sat} - CA) + \frac{\partial (WS_{CACO3} \cdot CACO3)}{\partial Z} \quad (79)$$

rKa: reaeration rate for CO2 (m/day)

CO_{2sat}: saturation concentration of CO2 (mg/L)

CO₂: aqueous carbon dioxide concentration (mg/L)

rKCACO₃: the dissolution/formation rate of calcium carbonate (day⁻¹)

CA_{sat}: the saturation concentration of dissolved calcium (mg [CACO₃]/L)

CA: the concentration of dissolved calcium (mg [CACO₃]/L)

mC: mole weight for carbon (=12.011 g)

mCACO₃: mole weight for calcium carbonate (=100.086 g)

mN: mole weight for calcium carbonate (=14.007 g)

CACO₃: the concentration of calcium carbonate (mg [CACO₃]/L)

WS_{CACO₃}: the settling velocity of calcium carbonate (m/day)

6.5 SAV Model

This part is still under development by Nicole Cai.

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