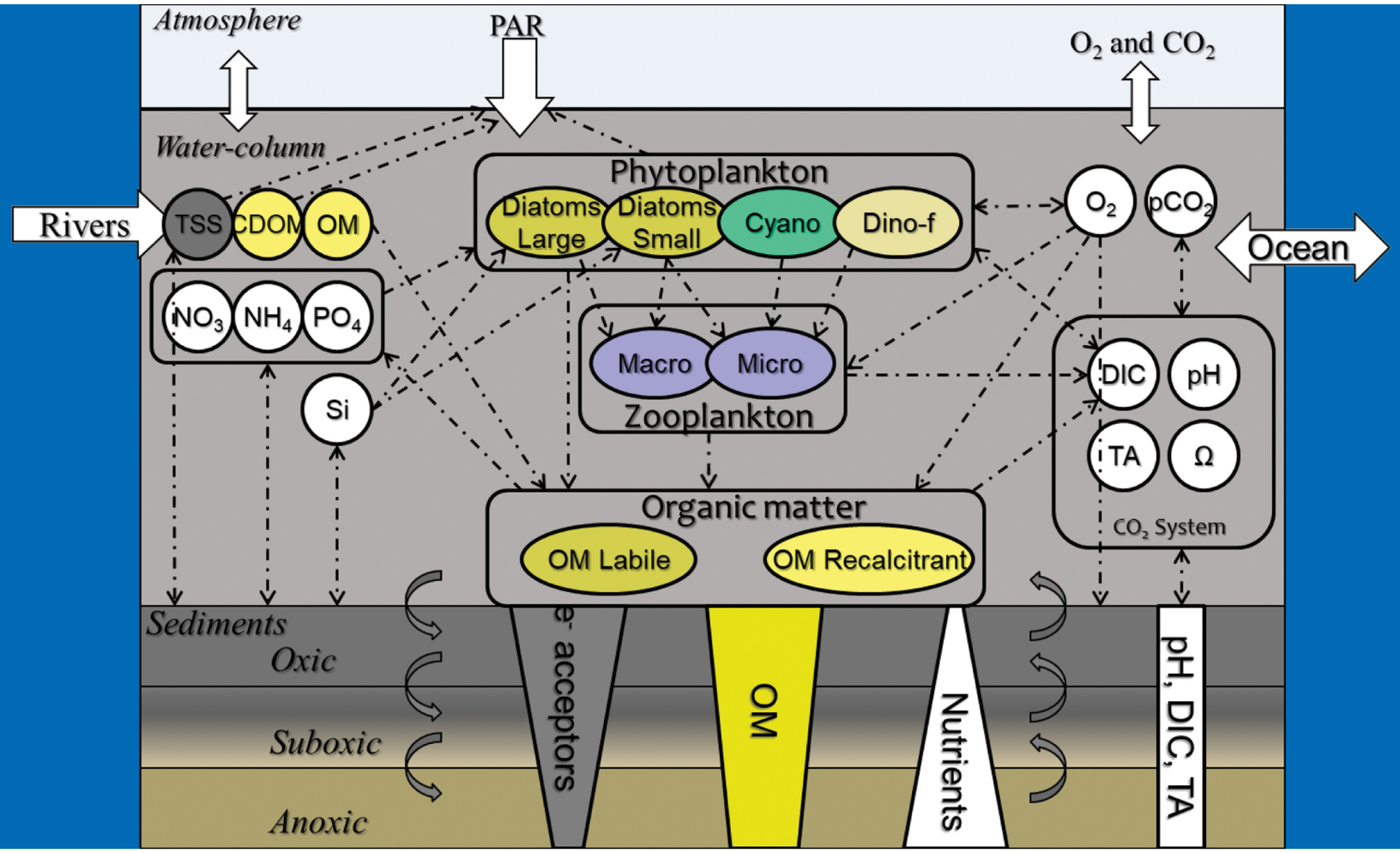
EPA/600/B-23/215| September 2023 | www.epa.gov/ord

United States Environmental Protection Agency

Coastal Generalized Ecosystem Model (CGEM)

VERSION 1.0

USER GUIDE



Office of Research and Development
Center for Environmental Measurement and Modeling

EPA/600/B-23/215 | September 2023 | www.epa.gov/ord

Coastal Generalized Ecosystem Model (CGEM)

VERSION 1.0
USER GUIDE

U.S. EPA Office of Research and Development
Center for Environmental Measurement and Modeling

Authors and Reviewers

Federal Authors

Brandon Jarvis, M.S.
U.S. EPA
Office of Research and Development
Center for Environmental Measurement and Modeling (CEMM)
Gulf Breeze, Florida

James Pauer, Ph.D.
U.S. EPA
Office of Research and Development
Center for Computational Toxicology and Exposure (CCTE)
Duluth, MN

Contract Authors

Cody Simmons, Ph.D.
Wilson Melendez, Ph.D.
General Dynamics Information Technology
US EPA, 109 T.W. Alexander Dr.
Research Triangle Park, NC 27711

Support for CGEM provided by

U.S. EPA Office of Research and Development

This User Guide was created under the Agency's Quality Assurance (QA) program for environmental information, with an approved Quality Assurance Project Plan (QAPP) for Enhancements to Coastal Generalized Ecosystem Model (CGEM), L-HEEAD-0032189-QP-1-2 (approved 9/30/2022).

Contents

Abbreviations

CGEM	Coastal Generalized Ecosystem Model
DIC	Dissolved Inorganic Carbon
DIN	Dissolved Inorganic Nitrogen
DIP	Dissolved Inorganic Phosphorus
DOC	Dissolved Organic Carbon
DOP	Dissolved Organic Phosphorus
DON	Dissolved Organic Nitrogen
DSi	Dissolved Silica
EFDC	Environmental Fluid Dynamics Code
FVCOM	Finite Volume Community Ocean Model
GOMDOM	Gulf of Mexico Dissolved Oxygen Model
HYCOM	Hybrid Coordinate Ocean Model
LOC	Labile Organic Carbon
LON	Labile Organic Nitrogen
LOP	Labile Organic Phosphorus
ROC	Refractory Organic Carbon
RON	Refractory Organic Nitrogen
WQEM	Water Quality Eutrophication Model

1.0 Overview

The U.S. Environmental Protection Agency (EPA) Coastal Generalized Ecosystem Model (CGEM) is a dynamic three-dimensional ecosystem model with functionality to simulate biogeochemical processes of coastal, estuarine, and freshwater ecosystems. Originally developed to address hypoxia in the northern Gulf of Mexico, CGEM has been adapted for implementation in a diverse range of aquatic ecosystems using customizable spatial and temporal resolutions. The CGEM codebase includes numerous formulation options for simulating ecosystem processes and also provides optional model kinetics used in the LM3 and Gulf of Mexico Dissolved Oxygen Model (GoMDOM) eutrophication models, hereafter referred to as the Water Quality Eutrophication Model (WQEM).

CGEM includes unlimited number of phytoplankton and zooplankton functional types, six classes of organic matter, and a state-of-the-art optical model for computing light attenuation based on inherent optical properties. CGEM also utilizes Droop nutrient kinetics, offering flexible internal cell nutrient quotas and uptake rates for more realistic phytoplankton nutrient limitation. CGEM includes an optional sediment diagenesis model for simulation of oxygen and nutrient fluxes from sediments, as well as simulation of carbonate chemistry (including pH, DIC, and alkalinity) for acidification and climate change analysis. As open-source code CGEM allows users to add or modify CGEM formulations as required and provides easy access to data via open-source NetCDF formats. CGEM also includes a utility facilitating linkage with the commonly applied EPA's Environmental Fluid Dynamics Code (EFDC) hydrodynamic model. The CGEM model is also parallelized to improve mode runtime performance.

1.1 What is CGEM

CGEM is a parallelized community ecosystem model that includes multiple biogeochemical formulations that can be run with the following options:

- 0D – a user-defined single cell
- 1D – a vertical column of cells
- 2D – an area of cells (single cell depth)
- 3D – a fully 3-dimensional volume of cells

CGEM was designed to address eutrophication, dissolved oxygen, and acidification dynamics in coastal and freshwater ecosystems. CGEM simulates biogeochemical processes regulating carbon, oxygen, nutrients, phytoplankton and zooplankton, and includes numerous model formulations and variable phytoplankton functional types that can be modified based on site specific model requirements. CGEM also includes a full sediment diagenesis model as well as formulations representing carbonate chemistry and pH necessary to address acidification and global climate change.

1.2 Water Quality Models Included in CGEM

CGEM includes two water quality modules that are available to the user within a single codebase. Users can switch between CGEM and WQEM model formulations based on specific modeling needs.

1.2.1 CGEM

CGEM is a biogeochemical, lower trophic level ecosystem model that simulates the biogeochemical processes regulating carbon, oxygen, nutrients, phytoplankton, and

zooplankton state variables. CGEM is based on the biogeochemical equations described in Eldridge and Roelke (2010). CGEM utilizes Droop nutrient kinetics and includes multiple phytoplankton and zooplankton functional types, four classes of organic matter in particulate and dissolved forms, and numerous formulation options for water column and sediment processes. A full description of CGEM, including state variables and model formulations, is provided in the CGEM Model Theory documentation.

1.2.2 WQEM

WQEM is an advanced eutrophication model developed based on the kinetic equations used in the he Corps of Engineers Water Quality Integrated Compartment Model (CE-QUAL-ICM) (Cerco and Cole, 1995). WQEM simulates 18 primary state variables that are common to both Monod and Droop kinetics, 4 Droop-specific state variables, and 1 tracer state variable. A full description of state variables and kinetic equations used in WQEM are provided in the WQEM Model Theory Documentation.

1.3 Hydrodynamic Models Usable by CGEM

1.3.1 EFDC

The Environmental Fluid Dynamics Code (EFDC) is a multifunctional surface water modeling system. EFDC has been applied to over 100 water bodies including rivers, lakes, reservoirs, wetlands, estuaries, and coastal ocean regions in support of environmental assessment and management and regulatory requirements.

EFDC is a state-of-the-art hydrodynamic model that can be used to simulate aquatic systems in one, two, and three dimensions. It has evolved over the past two decades to become one of the most widely used and technically defensible hydrodynamic models in the world. EFDC uses stretched or sigma vertical coordinates and Cartesian or curvilinear, orthogonal horizontal coordinates to represent the physical characteristics of a waterbody. It solves three-dimensional, vertically hydrostatic, free surface, turbulent averaged equations of motion for a variable-density fluid. Dynamically coupled transport equations for turbulent kinetic energy, turbulent length scale, salinity and temperature are also solved. The EFDC model allows for drying and wetting in shallow areas by a mass conservation scheme. The EFDC model and associated user documentation are available for download online (https://www.epa.gov/ceam/environmental-fluid-dynamics-code-efdc).

1.4 Other Included Models

1.4.1 Sediment Diagenesis Model (SDM)

CGEM includes an optional sediment diagenesis model by Eldridge and Roelke (2010). The diagenesis equations are run in parallel for the water quality model for simulation of benthic organic matter mineralization, including nutrient, oxygen, and carbonate fluxes.

1.5 About This User Guide

The aim of this user guide is to get you up and running with the CGEM code.

CGEM is a project under active and ongoing development, and uses a mix of Linux, Windows, and open-source technologies, such as Git and R.

A description of model formulations and equations is provided in separate documentation. This guide will not describe the scientific research supporting the codes.

1.6 How EPA Uses CGEM

EPA developed CGEM as a state-of-the-art water quality model to assess northern Gulf of Mexico hypoxia and to predict ecosystem response to reduced nutrient scenarios. These efforts have resulted in numerous publications that address a range of topics related to eutrophication and hypoxia in the northern Gulf of Mexico and beyond, including:

- Effects of nutrient boundaries on primary production (Pauer et. al., 2016)
- Effects of model boundary conditions and river loads on hypoxia (Feist et. al., 2017)
- Model parameter sensitivity and identifiability (Beck et. al., 2018)
- Effects of model boundary conditions and river loads on hypoxia (Feist et. al., 2017)
- Effects of climate change on Gulf hypoxia (Lehrter et. al., 2017)
- Spatiotemporal carbon dynamics controlling hypoxia (Jarvis et. al., 2020)
- Impact of model structure on simulation of hypoxia (Pauer et. al., 2020)
- Hypoxic zone effects on State water quality (Jarvis et. al., 2021)
- Intermodel comparison of simulated nutrient load reduction response (Jarvis et. al., 2022)
- Nearshore phosphorus dynamics in Lake Ontario (Pauer et. al., 2022)
- Diel oxygen dynamics in shallow estuaries (Jarvis et. al., 2023 [in review])

Future CGEM development and application will include integration with the U.S. Navy's Hybrid Coordinate Ocean Model (HYCOM) to address climate change effects on northern Gulf of Mexico hypoxia.

1.7 History of CGEM Development

CGEM's initial development began in 2009 as a tool for EPA to assess Gulf hypoxia and help inform nutrient management policy. CGEM was originally developed using the model of Eldridge and Roelke (2010), with numerous critical updates including dynamic time-variable computation and application of the model to a three-dimensional grid.

Since its inception CGEM has been applied to evaluate spatiotemporal hypoxia dynamics and the underlying mechanisms governing formation and maintenance of the seasonal hypoxic zone.

CGEM and WQEM have also been utilized for a comparison of model performance and outcomes in forecasting ecosystem recovery from proposed nutrient management policies.

In 2015 the CGEM model code was adapted for implementation beyond the Gulf of Mexico in formats ranging from steady state 0-dimensional models to full 3-dimensional models indirectly coupled to EFDC hydrodynamics.

In 2020 this new model code was parallelized to improve model runtime performance. Initial public release of CGEM includes all advancements in model formulations and code performance updates to allow full functionality and flexibility to the user.

1.8 What's New in CGEM 2.1

Initial public release of CGEM and associated utilities includes all available model updates to date. Future releases of updated versions will include expanded descriptions of added functionality.

1.9 Citing CGEM Results

We suggest the following for citing CGEM:

> CGEM (Coastal Generalized Ecosystem Model) is a biogeochemical, lower trophic level ecosystem model based on the biogeochemical equations described in Eldridge and Roelke (2010) with enhancements including a sediment diagenesis model, equations governing carbonate chemistry, and linkage with Environmental Fluid Dynamics Code (EFDC) hydrodynamic models.
>
> Eldridge, P. M., and Roelke, D. L. (2010). Origins and scales of hypoxia on the Louisiana shelf: Importance of seasonal plankton dynamics and river nutrients and discharge, Ecological Modelling, 221, 1028-1042, http://dx.doi.org/10.1016/j.ecolmodel.2009.04.054,

1.10 CGEM Resources

1.10.1 CGEM Website

CGEM is available for download from the Center for Exposure Assessment Modeling (CEAM) website.

1.10.2 CGEM Support

Technical support for CGEM, including questions regarding source code, utilities, and documentation, should be submitted through the Center for Exposure Assessment Modeling (CEAM) website.

2.0 Getting and Building CGEM

2.1 System Requirements

- Linux operating system
- Fortran compiler (either Intel or GNU Fortran compilers are recommended)
  - Currently using Intel 18.0.2 and IntelMPI v5.0.3.049 on Atmos
- NetCDF v4 or greater (https://downloads.unidata.ucar.edu/netcdf/)
  - CGEM currently uses NetCDF v4.6.3 on Atmos
- PnetCDF (for parallel compilation)
  - CGEM currently uses pNetCDF v1.9.0 on Atmos

2.2 Download CGEM source code

CGEM source code is available for download from the CGEM GitHub repository at https://github.com/USEPA/CGEM. Accessing the code requires a GitHub account.

2.2.1 Download as a zip file

A zip file of the source code is available at https://github.com/USEPA/CGEM/archive/refs/heads/master.zip.

2.2.2 Clone GitHub Repository

The Git repository may be cloned by using:

https://github.com/USEPA/CGEM.git for HTTPS

or

git@github.com:USEPA/CGEM.git for SSH

2.2.3 Latest Release Package

The latest full release package of the source code can be downloaded from the EPA CEAM website.

2.3 Compilation

2.3.1 Serial Compilation

Use the Makefile_serial_gen file as a template.

1. Modify Makefile_serial_gen as needed for your specific compiler, libraries, etc. in the "User Modifiable Section" of the makefile. The following examples are for both Intel and GNU Fortran compilers:
   - F90 – specify compiler (ex., ifort, gfortran, etc)
   - INC – specify path(s) to NetCDF include files
   - LIBS – specify path(s) to NetCDF libraries
   - FFLAGS – specify compiler flags as needed
2. Run the command "make -f Makefile_serial_gen" to compile.

Note **For Atmos users:** the files modules_intel.sh and modules_gfortran.sh will load the required modules for compilation for Intel and GNU compilers, respectively. Use the command "source <module_file>" to load the appropriate modules to your environment.

2.3.2 Parallel Compilation

Use the Makefile_par_gen file as a template.

1. Modify Makefile_par_gen as needed for your specific compiler, libraries etc in the "User Modifiable Section" of the makefile. The following example are for both Intel and GNU Fortran compilers:
   - F90 – specify compiler (ex., mpiifort, mpif90, etc)
   - INC – specify path(s) to NetCDF and PnetCDF include files
   - LIBS – specify path(s) to NetCDF and PnetCDF libraries
   - FFLAGS – specify compiler flags as needed
3. Run the command "make -f Makefile_par_gen" to compile.

Note **For Atmos users:** the files modules_intel.sh and modules_gfortran.sh will load the required modules for compilation for Intel and GNU compilers, respectively. Use the command "source <module_file>" to load the appropriate modules to your environment.

2.4 Troubleshooting

- If using the Linux package Modules, paths for include (INC) and library (LIBS) directories can be displayed using the command:

  module show <libraryname>

- For parallel compilations, specifying a number of tasks greater than the number of columns in the grid can cause errors. On Atmos, an example error message for this situation is

  PROBLEM: Failed to write output variable A1

  NetCDF: Index exceeds dimension bound

- If you have trouble, contact your local sysadmin (system administrator) for assistance.

3.0 Model Inputs and Switches

CGEM includes multiple switch options for setting formulation options related to sediment processes and phytoplankton growth parameters. Detailed information regarding these switch options is provided in the model framework documents for CGEM and WQEM.

3.1 Required Input Files

User-provided input file
Input file settings for phytoplankton and zooplankton are assigned as tab-spaced entries based on the number of phytoplankton (nospA) and zooplankton (nospZ), with phytoplankton entries made first.

For example, if nospA=3 and nospZ=2, three tab-spaced values should be entered for each phytoplankton parameter under phytoplankton section of the input file and two tab-spaced values for each zooplankton parameter in the zooplankton section.

Temperature settings for phytoplankton and zooplankton are entered in the temperature section as phytoplankton first followed by zooplankton.

For the previous example, there should be five tab-spaced entries for each parameter value, first three for phytoplankton, and the last two for zooplankton.

Initial Conditions File

Model_dim.txt File

Basic Grid

- Dat Files
  - d.dat – specifies depth from surface to bottom of cell in the 0-D model
  - dxdy.dat – specifies grid cell size
  - nz.dat – specifies number of cells in k-dir
  - T.dat (if using Read_T = 0, see Input File Setting) – specifies information for calculating temperature
  - /Input/Temp.dat (if using Read_T = 1, see Input File Setting) – specifies temperature data to be read
  - S.dat (if using Read_Sal = 0, see Input File Setting) – specifies constant salinity value
  - /Input/Sal.dat (if using Read_Sal = 1, see Input File Setting) – specifies salinity data to be read
  - /Input/Solar.dat (if using Read_Solar = 1, see Input File Setting) – specifies solar data to be read
  - /Input/Wind.dat (if using Read_Wind = 1, see Input File Setting) – specifies wind data to be read

EFDC Hydro

- Dat Files
  - dxdy.dat - specifies grid cell size
  - latlon.dat – specifies latitude and longitude for each grid cell
  - mask.dat – specifies land/water mask
  - nz.dat - specifies number of cells in k-dir
- NetCDF Files
  - Ev.nc – diffusivity coefficients data
  - Salt.nc – salinity data
  - SurfaceElev.nc

- Temp.nc – temperature data
- UFlow.nc – current flux data in i-direction
- VFlow.nc – current flux data in j-direction
- WFlow.nc – current flux data in k-direction
- WaterDepth.nc – column depth data
- LayerDepth.nc – layer depth data

Boundary Concentrations for CGEM (optional for EFDC Hydro)

- BCindices.dat
- /INPUT/TN_BoundaryConcentrations.nc
- /INPUT/NO3_BoundaryConcentrations.nc
- /INPUT/NH4_BoundaryConcentrations.nc
- /INPUT/DON_BoundaryConcentrations.nc
- /INPUT/TP_BoundaryConcentrations.nc
- /INPUT/DIP_BoundaryConcentrations.nc
- /INPUT/DOP_BoundaryConcentrations.nc
- /INPUT/BOD_BoundaryConcentrations.nc
- /INPUT/DO_BoundaryConcentrations.nc

River Loadings CGEM (optional for EFDC Hydro)

- RiverIndices.dat
- RiverWeights.dat
- /INPUT/TN_RiverLoads.nc
- /INPUT/NO3_RiverLoads.nc
- /INPUT/NH3_RiverLoads.nc
- /INPUT/DON_RiverLoads.nc
- /INPUT/TP_RiverLoads.nc
- /INPUT/DIP_RiverLoads.nc
- /INPUT/DOP_RiverLoads.nc
- /INPUT/BOD1_RiverLoads.nc
- /INPUT/DO_RiverLoads.nc

Boundary Concentrations for WQEM (optional for EFDC Hydro)

- BCindices.dat
- /INPUT/NO3_BoundaryConcentrations.nc
- /INPUT/NH4_BoundaryConcentrations.nc
- /INPUT/DON_BoundaryConcentrations.nc
- /INPUT/TP_BoundaryConcentrations.nc
- /INPUT/DIP_BoundaryConcentrations.nc
- /INPUT/DOP_BoundaryConcentrations.nc
- /INPUT/DO_BoundaryConcentrations.nc

River Loadings WQEM (optional for EFDC Hydro)

- /INPUT/TP_RiverLoads.nc
- /INPUT/NO3_RiverLoads.nc
- /INPUT/NH4_RiverLoads.nc
- /INPUT/DON_RiverLoads.nc
- /INPUT/DIP_RiverLoads.nc
- /INPUT/DOP_RiverLoads.nc
- /INPUT/DO_RiverLoads.nc

3.2 Input File Settings

3.2.1 CGEM Input File

Table 1. *Simulation Specifics*

Line#	Variable	Description
4	Starting time	year, month, day, hour, minute, second
5	Ending time	year, month, day, hour, minute, second
6	Timesteps	dT (timestep in seconds), dT_out (output interval in seconds), dT_sed (sediment diagenesis timestep in seconds)

Table 2. *Switches in CGEM*

Line#	Variable	Description
9	Which_fluxes	on ==1, off == 0: O2 surface, DIC surface, Sediment Oxygen Consumption, Microphytobenthos, Sediment Nutrient Fluxes, Atmospheric Deposition of Nutrients, Instant Remineralization in Bottom of Layer, Sediment Diagenesis Model
11	Which_temperature	1 == Sigmoidal, 2 == Optimum Temperature Threshold, 3 == Arrenhius, 4 == WQEM
12	Which_uptake	Nutrient uptake rate: 1 == Michaelis-Menten, 2 == Geider (needs nfQs), 3 == Roelke
13	Which_quota	Nutrient dependent growth: 1 == Droop, 2 == Nyholm, 3 == Flynn, 4 == WQEM
14	Which_irradiance	1 == IOP(inherent optical properties), 2 == AOP (apparent optical properties), 3 == WQEM
15	Which_chlaC	1 == fixed C:Chl-a, 2 == Cloern Chl:C
16	Which_photosynthesis	1 == photoinhibition, 2 == without photoinhibition, 3 == nutrient dependent, 4 == WQEM

Line#	Variable	Description
17	Which_growth	Specific growth rate: 1 == minimum, 2 == product formulation, 3 == umax is nutrient dependent
18	ReadVars	Solar – Calculate(0)/Read(1), Wind – 5mph(0)/Read(1), Temperature – cosine with parameters(0)/Read(1), Salinity – Read one value(0)/Read(1)
19	InitializeHow	0 == Read File, 1 == Salinity Regression

Table 3. *Optics*

Line#	Variable	Description
22	Kw	AOP, light attenuation due to water
23	Kcdom	AOP, light attenuation due to CDOM
24	Kspm	AOP, light attenuation due to SPM
25	Kchla	AOP, light attenuation due to chla
26	Astar490	Chla specific absorption at 490 nm
27	Aw490	seawater absorption at 490 nm
28	astarOMA	OM_A specific absorption at 490 nm
29	astarOMZ	OM_Z specific absorption at 490 nm
30	astarOMR	OM_R specific absorption at 490 nm
31	astarOMBC	OM_BC specific absorption at 490 nm
32	PARfac	Multiplies surface PAR
33	Sink CDOM	sinking rate

Table 4. *Temperature*

Line#	Variable	Description
36	Tref	(nospA + nospZ) – Optimum temperature for growth (°C)
37	KTg1	(nospA + nospZ) – Effect of T below Topt ($°C^2$)
38	KTg2	(nospA + nospZ) – Effect of T above Topt ($°C^2$)
39	Ea	(nospA + nospZ) – Slope of Arrhenius plot (eV)

Table 5. *Phytoplankton (up to six types)*

Line#	Variable	Description
42	edibleVector (Z1)	edibility vector for Z1
43	edibleVector (Z2)	edibility vector for Z2
44	umax	maximum growth rate

Line#	Variable	Description
45	Fixed C	Chla ratio
46	alpha	initial slop of the photosynthesis/irradiance relationship
47	beta	photoinhibition constant
48	respg	phytoplankton growth respiration coefficient
49	respb	phytoplankton basal respiration coefficient
50	QminN	minimum N cell-quota
51	QminP	minimum P cell-quota
52	QmaxN	maximum N cell-quota
53	QmaxP	maximum P cell-quota
54	Kn	half-saturation constant for N
55	Kp	half-saturation constant for P
56	Ksi	half-saturation constant for Si uptake
57	kQn	Qn constant for Flynn nutrient dependent growth model
58	kQp	Qp constant for Flynn nutrient dependent growth model
59	nfQs	exponent for Geider nutrient uptake model
60	vmaxN	N-uptake rate measured at umax
61	vmaxP	P-uptake rate measured at umax
62	vmaxSi	Si-uptake rate measured at umax
63	aN	coefficient for non-limiting nutrient
64	volcell	phytoplankton volume/cell
65	Qc	phytoplankton carbon/cell
66	Athresh	phytoplankton threshold for grazing (is multiplied by volcell)
67	sink A	sinking rate of phytoplankton cells
68	mA	mortality coefficient
69	A_wt	relative proportion of total chlA for initializing phytoplankton

Table 6. *Zooplankton (up to two types)*

Line#	Variable	Description
72	Zeffic	assimilation efficiency as a fraction of ingestion
73	Zslop	proportion of grazed phytoplankton lost to sloppy feeding
74	Zvolcell	zooplankton volume/individual
75	ZQc	zooplankton carbon/individual
76	ZQn	zooplankton nitrogen/individual
77	ZQp	zooplankton phosphorus/individual
78	Zka	half saturation coefficient for grazing

Line#	Variable	Description
79	Zrespg	zooplankton growth-dependent respiration factor
80	Zrespb	zooplankton biomass-dependent respiration factor
81	Zumax	maximum growth rate of zooplankton
82	Zm	zooplankton mortality constant for quadratic mortality

Table 7. *Organic Matter*

Line#	Variable	Description
85	KG1	turnover rate for OM1_A and OM1_Z
86	KG2	turnover rate for OM2_A and OM2_Z
87	KG1_R	OM1 turnover rate for riverine
88	KG2_R	OM2 turnover rate for riverine
89	KG1_BC	OM1 turnover rate for initial and bc
90	KG2_BC	OM2 turnover rate for initial and bc
91	KNH4	NHV rate constant for nitrification
92	nitmax	maximum rate of nitrification per day
93	KO2	half-saturation concentration for O2 utilization
94	KstarO2	O2 concentration that inhibits denitrification
95	KNO3	half-saturation concentration for NO3 used in denitrification
96	pCO2	atmospheric CO2
97	stoich_x1R	C:P stoichiometry of OM1_R
98	stoich_y1R	N:P stoichiometry of OM1_R
99	stoich_x2R	C:P stoichiometry of OM2_R
100	stoich_y2R	N:P stoichiometry of OM2_R
101	stoich_x1BC	C:P stoichiometry of OM1_BC
102	stoich_y1BC	N:P stoichiometry of OM1_BC
103	stoich_x2BC	C:P stoichiometry of OM2_BC
104	stoich_y2BC	N:P stoichiometry of OM2_BC
105	sink OM1_A	sinking rate
106	sink OM2_A	sinking rate
107	sink OM1_Z	sinking rate
108	sink OM2_Z	sinking rate
109	sink OM1_R	sinking rate
110	sink OM2_R	sinking rate
111	sink OM1_BC	sinking rate
112	sink OM2_BC	sinking rate

Line#	Variable	Description
113	Kgcdom	decay rate of CDOM, 1/day
114	CF_SPM	conversion factor for river OM to river SPM

Table 8. *Other, Including Boundary Conditions*

Line#	Variable	Description
117	Which_Vmix/Adv	0 == No Vmixing/Adv, 1 == Yes VMixing/Adv
118	KH_coeff	multiplying factor for KH in VMixing
119	Which_Outer_BC	0 == salinity, 1 == zero nutrients at lateral bc, 2 == zero nutrients lateral and open ocean, 3 == small gradient, 4 == WQEM, 5 == no flow boundaries, 6 == salinity with depth attenuation
121	wt_pl, wt_po	weights for plankton at the lateral and open ocean, Set 1 for normal salinity BCs
122	wt_l, wt_o	weights for small gradient BCs, lateral and open ocean
123	OM_BC multipliers	multipliers for OM_BC at initial conditions and for boundary conditions, lateral and shelf
124	Stoich_x1_init, Stoich_y1_init	initial stoichiometry of all OM1_A
125	Stoich_x2_init, Stoich_y2_init	initial stoichiometry of all OM2_A
126	Stoich_x1Z_init, Stoich_y1Z_init	initial stoichiometry of all OM1_Z
127	Stoich_x2Z_init, Stoich_y2Z_init	initial stoichiometry of all OM2_Z
128	KG_bot	turnover rate for k=20 if Instant Remineralization is used (see Which_fluxes in Table 2)
129	MC	0 == No daily integrated rates output, 1 == Yes daily integrated rates output
130	Which_Output	0 == normal output, 1 == NRL, 2 == ALL_FALSE

3.2.2 WQEM Input File

Table 9. *Simulation Specifics*

Line#	Variable	Description
4	Starting time	year, month, day, hour, minute, second (YYYY M D h m s)
5	Ending time	year, month, day, hour, minute, second (YYYY M D h m s)
6	Timesteps	dT (timestep in seconds), dT_out (output interval in seconds), dT_sed (sediment diagenesis timestep in seconds)

Table 10. *Switches in GEM*

Line#	Variable	Description
9	Which_fluxes	on ==1, off == 0: O2 surface, DIC surface, Sediment Oxygen Consumption, Microphytobenthos, Sediment Nutrient Fluxes, Atmospheric Deposition of Nutrients, Instant Remineralization in Bottom of Layer (1==with Flux, 2==just sinking), Sediment Diagenesis Model, Silica
11	ReadVars	Solar – Calculate(0)/Read(1)/Read PAR(2), Wind – 5mph(0)/Read(1), Temperature – cosine with parameters(0)/Read(1), Salinity – Read one value(0)/Read(1)
12	InitializeHow	0 == Read File, 1 == Salinity Regression

Table 11. *Optics*

Line#	Variable	Description
15	Which_irradiance	0 == None, 1 == WQEM, 2 == Inherent Optical Properties
16	Astar490	Chla specific absorption at 490 nm (m^{-1} (mg Chla m^{-3})$^{-1}$)
17	Aw490	seawater absorption at 490 nm (m^{-1})
18	astarOMA	OM_A specific absorption at 490 nm (m^{-1})
19	astarOMZ	OM_Z specific absorption at 490 nm (m^{-1})
20	astarOMR	OM_R specific absorption at 490 nm (m^{-1})
21	astarOMBC	OM_BC specific absorption at 490 nm (m^{-1})
22	PARfac	Multiplies surface PAR

Table 12. *River Loads (used in 3D only)*

Line#	Variable	Description
25	rcNO3	factor multiplying NO3 river load
26	rcHN4	factor multiplying NH4 river load
27	rcPO4	factor multiplying PO4 river load
28	rcSi	factor multiplying Si river load

Table 13. *Other including Boundary Conditions*

Line#	Variable	Description
31	Which_Vmix	0 == No Vertical Mixing, 1 == Vertical Mixing is on
32	KH_coeff	Scaling factor for vertical mixing coefficients (KH).
33	Which_Outer_BC	0 == Salinity, 1== WQEM original, 2 == WQEM Full Grid
34	DoDroop	0 == No Droop kinetics, 1 == Droop kinetics
40	ALPHA_DIA	Initial slope of diatom's light saturation curve (g C (g Chl a)$^{-1}$ h^{-1} (umol quanta)$^{-1}$ m^{-2} s^{-1})
41	ALPHA_GRE	Initial slope of greens' light saturation curve (g C (g Chl a)$^{-1}$ h^{-1} (umol quanta)$^{-1}$ m^{-2} s^{-1})
43	ANCP	N:C ratio for plankton
44	APCP	P:C ratio for plankton
45	ASCD	Si:C ratio for diatoms
46	AVFRAC	Available fraction of DOP
47	AVFRACDON	Available fraction of DON
49	BMRD	Diatom base metabolic rate (s^{-1})
50	BMRG	Non-Diatom algae base metabolic rate (s^{-1})
52	CCHLD	Carbon:chlorophyll ratio for diatoms
53	CCHLG	Carbon:chlorophyll ratio for non-diatom algae
55	CGZ	Zooplankton maximum growth rate (s^{-1})
57	DENIT_CN_RATIO	Denitrification C:N ratio
59	GCDD	Fraction of basal metabolism exuded as DOC by diatoms
60	FCDG	Fraction of basal metabolism exuded as DOC by non-diatoms
61	FCDP	Fraction of DOC produced by predation
62	FCDZ	Fraction of DOC from zooplankton mortality
63	FCLD	Fraction of labile POC produced by diatoms metabolism
64	FCLG	Fraction of labile POC produced by non-diatoms metabolism
65	FCLP	Fraction of labile PDC from predation
66	FCLZ	Fraction of labile PDC from zooplankton mortality
67	FCRD	Fraction of refractory POC produced by diatoms metabolism
68	FCRG	Fraction of refractory POC produced by non-diatoms metabolism
69	FCRP	Fraction of refractory PDC from predation
70	FCRZ	Fraction of refractory PDC from zooplankton mortality
71	FNDD	Fraction of DON produced by diatom metabolism

Line#	Variable	Description
72	FNDG	Fraction of DON produced by non-diatom algae metabolism
73	FNDP	Fraction of DON produced by predation
74	FNDZ	Fraction of DON produced by zooplankton mortality
75	FNID	Fraction of inorganic nitrogen produced by diatom metabolism
76	FNIG	Fraction of Inorganic nitrogen produced by non-diatom algae metabolism
77	FNIP	Fraction of inorganic nitrogen produced by predation
78	FNIZ	Fraction of inorganic nitrogen produced by zooplankton mortality
79	FNLD	Fraction of labile particulate nitrogen produced by diatom metabolism
80	FNLG	Fraction of labile particulate nitrogen produced by non-diatom algae metabolism
81	FNLP	Fraction of labile particulate nitrogen produced by predation
82	FNLZ	Fraction of LON produced by zooplankton mortality
83	FNRD	Fraction of refractory particulate nitrogen produced by diatom metabolism
84	FNRG	Fraction of refractory particulate nitrogen produced by non-diatom metabolism
85	FNRP	Fraction of RON produced by predation
86	FNRZ	Fraction of RON produced by zooplankton mortality
87	FPDD	Fraction of DOP produced by diatom metabolism
88	FPDG	Fraction of DOP produced by non-diatom algae metabolism
89	FPDP	Fraction of DOP produced by predation
90	FPDZ	Fraction of DOP produced by zooplankton mortality
91	FPID	Fraction of inorganic phosphorus produced by diatom metabolism
92	FPIG	Fraction of inorganic phosphorus produced by non-diatom algae metabolism
93	FPIP	Fraction of inorganic phosphorus produced by predation
94	FPIZ	Fraction of inorganic phosphorus produced by zooplankton mortality
95	FPLD	Fraction of LOP produced by diatom metabolism
96	FPLG	Fraction of LOP produced by non-diatom algae metabolism
97	FPLP	Fraction of LOP produced by predation
98	FPLZ	Fraction of LOP produced by zooplankton mortality
99	FPRD	Fraction of ROP produced by diatom metabolism
100	FPRG	Fraction of ROP produced by non-diatom algae metabolism
101	FPRP	Fraction of ROP produced by predation
102	FPRZ	Fraction of ROP produced by zooplankton mortality

Line#	Variable	Description
103	FSAP	Fraction of silica made available through predation
105	GREFF	Zooplankton grazing efficiency
107	ILMUL	Scaling factor for surface short wave radiation
109	KDC	Minimum DOC mineralization rate (s^{-1})
110	KDCALG	DOC mineralization rate algal dependence ($m^3\ kg^{-1}\ s^{-1}$)
111	KDN	Minimum DON mineralization rate (s^{-1})
112	KDNALG	DON mineralization rate algal dependence ($m^3\ kg^{-1}\ s^{-1}$)
113	KDP	Minimum DOP mineralization rate (s^{-1})
114	KDPALG	DOP mineralization rate algal dependence ($m^3\ kg^{-1}\ s^{-1}$)
116	KDWD	Specifies light attenuation equation: 0 == regression, 1 == ambient chlorophyll ()
117	KE	Background light attenuation (m^{-1})
118	KECHL	Light attenuation factor for chlorophyll a ($mg^2\ kg^{-1}$)
120	KHDONT_SED	Half-saturation concentration of dissolved oxygen required for nitrification in the sediment bed. (kg m^{-3})
121	KHN	Organic nitrogen decay half-saturation constant (kg m^{-3})
122	KHND	Mean half-saturation constant for nitrogen uptake by diatoms (kg m^{-3})
123	KHNG	Mean half-saturation constant for nitrogen uptake by non-diatom algae (kg m^{-3})
124	KHNNT	Half-saturation concentration of NH4 required for nitrification (kg m^{-3})
125	KHODOC_SED	Half-Saturation concentration of O2 required for oxic respiration in the sediment bed (kg m^{-3})
126	KHP	Organic phosphorus decay half-saturation constant (kg m^{-3})
127	KHPD	Mean half-saturation constant for diatom phosphorus uptake (kg m^{-3})
128	KHPG	Mean half-saturation constant for non-diatom algae phosphorus uptake (kg m^{-3})
129	KHSD	Mean half-saturation constant for diatom silica uptake (kg m^{-3})
130	KLC	Minimum hydrolysis rate of LOC (s^{-1})
131	KLCALG	LOC hydrolysis rate algal dependence ($m^3\ kg^{-1}\ s^{-1}$)
132	KLN	Minimum hydrolysis rate of LON (s^{-1})
133	KLNALG	LON hydrolysis rate algal dependence ($m^3\ kg^{-1}\ s^{-1}$)
134	KLP	Minimum hydrolysis rate of LOP (s^{-1})
135	KLPALG	LOP hydrolysis rate algal dependence ($m^3\ kg^{-1}\ s^{-1}$)
136	KRC	Minimum hydrolysis rate of ROC (s^{-1})
137	KRCALG	ROC hydrolysis rate algal dependence ($m^3\ kg^{-1}\ s^{-1}$)

Line#	Variable	Description
138	KRN	Minimum hydrolysis rate of RON (s^{-1})
139	KRNALG	RON hydrolysis rate algal dependence ($m^3\ kg^{-1}\ s^{-1}$)
140	KRP	Minimum hydrolysis rate of ROP (s^{-1})
141	KRPALG	ROP hydrolysis rate algal dependence ($m^3\ kg^{-1}\ s^{-1}$)
142	KSUA	Particulate silica dissolution rate constant (s^{-1})
143	KSZ	Half-saturation coefficient of zooplankton for phytoplankton (kg m^{-3})
144	KTBD	Metabolism temperature dependence factor for diatoms ($°C^{-1}$)
145	KTBG	Metabolism temperature dependence factor for non-diatoms ($°C^{-1}$)
146	KTGD1	Effect of temperature below optimal temperature for diatoms ($°C^{-2}$)
147	KTGD2	Effect of temperature above optimal temperature for diatoms ($°C^{-2}$)
148	KTGG1	Effect of temperature below optimal temperature for non-diatoms ($°C^{-2}$)
149	KTGG2	Effect of temperature above optimal temperature for non-diatoms ($°C^{-2}$)
150	KTHDR	Hydrolysis temperature dependence ($°C^{-1}$)
151	KTMNL	Mineralization temperature dependence ($°C^{-1}$)
152	KTNT1	Effect of temperature below optimal temperature nitrification ($°C^{-2}$)
153	KTNT2	Effect of temperature above optimal temperature for nitrification ($°C^{-2}$)
154	KTSUA	Silica dissolution temperature rate constant ($°C^{-1}$)
155	NTM	Nitrification rate coefficient at optimal temperatures (kg $m^{-3}\ s^{-1}$)
156	PBMAX_DIA	Photosynthetic rate of diatoms at optimum illumination (gC $[gChl\text{-}a]^{-1}\ h^{-1}$)
157	PBMAX_GRE	Photosynthetic rate of greens at optimum illumination (gC $[gChl\text{-}a]^{-1}\ h^{-1}$)
158	PMD	Diatom production under optimal conditions (s^{-1})
159	PMG	Non-diatom algae production under optimal conditions (s^{-1})
161	SILIM	Nutrient limitation: 1 == Minimum of N and P, 2 == Minimum of N, P, and Si, 3 == No minimum
163	TMD	Temperature of optimum growth for diatoms (°C)
164	TMG	Temperature of optimum growth for non-diatoms (°C)
165	TMNT	Optimal temperature for nitrification (°C)
166	TRD	Metabolism reference temperature for diatoms (°C)
167	TRG	Metabolism reference temperature for non-diatoms (°C)
168	TRHDR	Reference temperature for hydrolysis (°C)
169	TRMNL	Reference temperature for mineralization (°C)
170	TRSUA	Silica dissolution reference temperature (°C)

Line#	Variable	Description
171	TZREF	Predation reference temperature (°C)
172	ZDTH	Zooplankton death/die-off coefficient (s^{-1})
173	ZTHET	Temperature coefficient for predation

Table 14. *Dissolved Oxygen-Related Parameters*

Line#	Variable	Description
177	KCOD	COD oxidation rate (s^{-1})
178	KDENITR	Maximum denitrification rate coefficient (s^{-1})
179	KHDENITR	Half-saturation concentration of NO3 required for denitrification (kg m^{-3})
180	KHDONT	Half-saturation concentration of dissolved oxygen required for nitrification (kg m^{-3})
181	KHOCOD	Half-Saturation concentration of O2 required for exertion of chemical oxygen demand (kg m^{-3})
182	KHODOC	Half-Saturation concentration of O2 required for oxic respiration (kg m^{-3})
183	KRDO	Reaeration coefficient (m s^{-1})
184	RCDO	Dissolved Oxygen-to-Carbon ratio ((mol of O_2)/(mol of C))
185	RNTO	O_2:N conversion factor (kg O_2 (kg N)$^{-1}$)

Table 15. *Droop Kinetics (not used in Monod and not tested yet)*

Line#	Variable	Description
189	FINTNID	Fraction of inorganic nitrogen produced by diatoms metabolism
190	FINTNDD	Fraction of dissolved nitrogen produced by diatoms metabolism
191	FINTNLD	Fraction of labile nitrogen produced by diatoms metabolism
192	FINTNRD	Fraction of refractory nitrogen produced by diatoms metabolism
193	FINTNIG	Fraction of inorganic nitrogen produced by non-diatoms metabolism
194	FINTNDG	Fraction of dissolved nitrogen produced by non-diatoms metabolism
196	FINTNLG	Fraction of labile nitrogen produced by non-diatoms metabolism
197	FINTNRG	Fraction of refractory nitrogen produced by non-diatoms metabolism
199	FINTLUXNIP	Fraction of luxury inorganic nitrogen produced by predation
200	FINTSTRNIP	Fraction of structural inorganic nitrogen produced by predation
201	FINTLUXNDP	Fraction of luxury dissolved organic nitrogen produced by predation
202	FINTSTRNDP	Fraction of structural dissolved organic nitrogen produced by predation
203	FINTLUXNLP	Fraction of luxury labile nitrogen produced by predation
204	FINTSTRNLP	Fraction of structural labile nitrogen produced by predation
205	FINTLUXNRP	Fraction of luxury refractory nitrogen produced by predation

Line#	Variable	Description
206	FINTSTRNRP	Fraction of structural refractory nitrogen produced by predation
208	FINTPID	Fraction of inorganic phosphorus produced by diatoms metabolism
209	FINTPDD	Fraction of dissolved phosphorus produced by diatoms metabolism
210	FINTPLD	Fraction of labile phosphorus produced by diatoms metabolism
211	FINTPRD	Fraction of refractory phosphorus produced by diatoms metabolism
213	FINTPIG	Fraction of inorganic phosphorus produced by non-diatoms metabolism
214	FINTPDG	Fraction of dissolved phosphorus produced by non-diatoms metabolism
215	FINTPLG	Fraction of labile phosphorus produced by non-diatoms metabolism
216	FINTPRG	Fraction of refractory phosphorus produced by non-diatoms metabolism
218	FINTLUXPIP	Fraction of luxury inorganic phosphorus produced by predation
219	FINTSTRPIP	Fraction of structural inorganic phosphorus produced by predation
220	FINTLUXPDP	Fraction of luxury dissolved organic phosphorus produced by predation
221	FINTSTRPDP	Fraction of structural dissolved organic phosphorus produced by predation
222	FINTLUXPLP	Fraction of luxury labile phosphorus produced by predation
223	FINTSTRPLP	Fraction of structural labile phosphorus produced by predation
224	FINTLUXPRP	Fraction of luxury refractory phosphorus produced by predation
225	FINTSTRPRP	Fraction of structural refractory phosphorus produced by predation
227	KHINTND	Half-saturation concentration for nitrogen uptake in diatoms (kg m^{-3})
228	KHINTNG	Half-saturation concentration for nitrogen uptake in non-diatoms (kg m^{-3})
229	KHINTPD	Half-saturation concentration for phosphorus uptake in diatoms (kg m^{-3})
230	KHINTPG	Half-saturation concentration for phosphorus uptake in non-diatoms (kg m^{-3})
232	QMINND	Minimum nitrogen quota for diatoms (kg N kg^{-1} algal C)
233	QMINNG	Minimum nitrogen quota for non-diatoms (kg N kg^{-1} algal C)
234	QMINPD	Minimum phosphorus quota for diatoms (kg N kg^{-1} algal C)
235	QMINPG	Minimum phosphorus quota for non-diatoms (kg N kg^{-1} algal C)
236	QMAXND	Maximum nitrogen quota for diatoms (kg N kg^{-1} algal C)
237	QMAXNG	Maximum nitrogen quota for non-diatoms (kg N kg^{-1} algal C)
238	QMAXPD	Maximum phosphorus quota for diatoms (kg N kg^{-1} algal C)
239	QMAXPG	Maximum phosphorus quota for non-diatoms (kg N kg^{-1} algal C)

Line#	Variable	Description
240	UPNMAXD	Maximum uptake rate of nitrogen by diatoms (kg N kg^{-1} algal C s^{-1})
241	UPNMAXG	Maximum uptake rate of nitrogen by greens (kg N kg^{-1} algal C s^{-1})
242	UPPMAXD	Maximum uptake rate of phosphorus by diatoms (kg P kg^{-1} algal C s^{-1})
243	UPPMAXG	Maximum uptake rate of phosphorus by greens (kg P kg^{-1} algal C s^{-1})

Table 16. *Settling Rates*

Line#	Variable	Description
247	VDIA	Settling rate for diatoms (m s^{-1})
248	VDIAN	Settling rate for diatom's internal nitrogen (m s^{-1})
249	VDIAP	Settling rate for diatom's internal phosphorus (m s^{-1})
250	VGRE	Settling rate for greens (m s^{-1})
251	VGREN	Settling rate for greens' internal nitrogen (m s^{-1})
252	VGREP	Settling rate for greens' internal phosphorus (m s^{-1})
253	VLOC	Settling rate for labile organic carbon (m s^{-1})
254	VROC	Settling rate for refractory organic carbon (m s^{-1})
255	VLON	Settling rate for labile organic nitrogen (m s^{-1})
256	VRON	Settling rate for refractory organic nitrogen (m s^{-1})
257	VLOP	Settling rate for labile organic phosphorus (m s^{-1})
258	VROP	Settling rate for refractory organic phosphorus (m s^{-1})
259	VSU	Settling rate for unavailable silica (m s^{-1})
260	VTR	Settling rate for tracer (m s^{-1})

3.3 ModelDim.txt

Table 17. *ModelDim.txt*

Line#	Variable	Description
2	IM	Number of cells in i direction
3	JM	Number of cells in j direction
4	nz_max	Max number of cells in k direction
5	nospA	Number of phytoplankton species
6	nospZ	Number of zooplankton species
7	Which_gridio	Hydrodynamic grid specification
8	iYr0	Start year for timestamps
9	Number of Rivers	Number of Rivers
10	Number of Boundary Cells	Number of Boundary Cells

3.4 Executable Command Line Arguments

Command line arguments can be used when calling the executable (Makefile default executable name is CGEM). You may omit arguments to use default settings. To specify any particular argument, all previous arguments must be specified. For example, to specify an initial conditions file (argument 3), the water quality model (argument 1) and input file (argument 2) must also be specified.

1. Argument 1 – User selected water quality model: Options are “CGEM” or “WQEM”
   - Default is “CGEM”
2. Argument 2 – User selected input file name (path relative to main CGEM directory). Defaults are:
   - “GEM_InputFile” for CGEM WQM
   - “WQEM_InputFile” for WQEM WQM
3. Argument 3 – User selected initial conditions file name (path relative to path located in MyFiles.inp). Defaults are:
   - “InitialConditions.txt” for CGEM WQM
   - “InitialConditions_WQEM.txt” for WQEM WQM
4. Argument 4 – User selected output file name (path relative to main CGEM directory). Defaults are:
   - “./NETCDF/cgem.” for CGEM WQM
   - “./NETCDF/wqem.” for WQEM WQM
5. Argument 5 – User selected Daily Integrated Rates filename (path relative to main CGEM directory):
   - Default is “./NETCDF/CGEM_DailyIntegrated_Rates.nc”

4.0 Model Output

4.1 CGEM

The model output of CGEM consists of two separate netcdf files. The default names of these files are CGEM_DailyIntegrated_Rates.nc and cgem.000000.nc.

The cgem.000000.nc file is always generated by default while the generation of CGEM_DailyIntegrated_Rates.nc can be turned on or off by setting the flag “MC” equal to 1 or 0 in the input deck, respectively.

Output file CGEM_DailyIntegrated_Rates.nc includes daily integrated model output regardless of the model output timestep included in cgem.000000.nc.

4.1.1 cgem.000000.nc

The variables stored in this netcdf file (assuming 3 phytoplankton and 2 zooplankton classes) are as follows.

Table 18. *cgem.000000.nc file variables*

Variable Name	Description	Units
LONGXY	Cell center longitude [-180, 180]	degrees
LATIXY	Cell center latitude [-90, 90]	degrees
h	Depth	m
fm	Mask: 0 = land, 1 = water	NA
dz	Thickness of cell	m
A1	Phytoplankton group 1 number density	organisms m^{-3}
A2	Phytoplankton group 2 number density	organisms m^{-3}
A3	Phytoplankton group 3 number density	organisms m^{-3}
Qn1	Phytoplankton group 1 nitrogen quota	mmol $cell^{-1}$
Qn2	Phytoplankton group 2 nitrogen quota	mmol $cell^{-1}$
Qn3	Phytoplankton group 3 nitrogen quota	mmol $cell^{-1}$
Qp1	Phytoplankton group 1 phosphorus quota	mmol $cell^{-1}$
Qp2	Phytoplankton group 2 phosphorus quota	mmol $cell^{-1}$
Qp3	Phytoplankton group 3 phosphorus quota	mmol $cell^{-1}$
Z1	Zooplankton group 1 number density	organisms m^{-3}
Z2	Zooplankton group 2 number density	organisms m^{-3}
NO3	Nitrate	mmol m^{-3}
NH4	Ammonium	mmol m^{-3}
PO4	Phosphate	mmol m^{-3}
DIC	Dissolved inorganic carbon	mmol m^{-3}
O2	Molecular oxygen	mmol m^{-3}

Variable Name	Description	Units
OM1_A	Particulate organic matter derived from dead algae	mmol m^{-3}
OM2_A	Dissolved organic matter derived from dead algae	mmol m^{-3}
OM1_Z	Particulate organic matter derived from zooplankton fecal pellets	mmol m^{-3}
OM2_Z	Dissolved organic matter derived from zooplankton fecal pellets	mmol m^{-3}
OM1_R	Particulate organic matter derived from river outflow	mmol m^{-3}
OM2_R	Dissolved organic matter derived from river outflow	mmol m^{-3}
CDOM	Colored dissolved organic matter	ppb
Si	Silica	mmol m^{-3}
OM1_BC	Particulate organic matter in the initial and boundary conditions	mmol m^{-3}
OM2_BC	Dissolved organic matter in the initial and boundary conditions	mmol m^{-3}
ALK	Alkalinity	mmol m^{-3}
Tr	Tracer should be =1	NA
irradiance	Irradiance at depth	photons cm^{-2} s^{-1}
irradiance_fraction	Fraction of surface irradiance	%
uN1	nitrogen-dependent growth rate for A1	d^{-1}
uN2	nitrogen-dependent growth rate for A2	d^{-1}
uN3	nitrogen-dependent growth rate for A3	d^{-1}
uP1	phosphorus-dependent growth rate for A1	d^{-1}
uP2	phosphorus-dependent growth rate for A2	d^{-1}
uP3	phosphorus-dependent growth rate for A3	d^{-1}
uE1	light-dependent growth rate for A1	d^{-1}
uE2	light-dependent growth rate for A2	d^{-1}
uE3	light-dependent growth rate for A3	d^{-1}
uA1	specific growth rate for A1	d^{-1}
uA2	specific growth rate for A2	d^{-1}
uA3	specific growth rate for A3	d^{-1}
Chla_mg_tot	Total Chla from all phytoplankton	mg m^{-3}
s_x1A	Stoichiometry C:P for OM1_A	mmol/mmol
s_y1A	Stoichiometry N:P for OM1_A	mmol/mmol
s_x2A	Stoichiometry C:P for OM2_A	mmol/mmol
s_y2A	Stoichiometry N:P for OM2_A	mmol/mmol
s_x1Z	Stoichiometry C:P for OM1_Z	mmol/mmol

Variable Name	Description	Units
s_y1Z	Stoichiometry N:P for OM1_Z	mmol/mmol
s_x2Z	Stoichiometry C:P for OM2_Z	mmol/mmol
s_y2Z	Stoichiometry N:P for OM2_Z	mmol/mmol
uSi1	silica-dependent growth rate for A1	d^{-1}
uSi2	silica-dependent growth rate for A2	d^{-1}
uSi3	silica-dependent growth rate for A3	d^{-1}
pH	pH	s.u.
RN2	RN2 Denitrification Term	mmol m^{-3}
RO2A	RO2A Decay Term	mmol m^{-3}
RO2Z	RO2Z Decay Term	mmol m^{-3}
RO2BC	RO2BC Decay Term	mmol m^{-3}
RO2R	RO2R Decay Term	mmol m^{-3}
Primary_Production	Primary Production	mmol m^{-3} d^{-1}

4.1.2 CGEM_DailyIntegrated_Rates.nc

Table 19. *CGEM_DailyIntegrated_Rates.nc file variables*

Variable Name	Description	Units
fm	Mask: 0 = land, 1 = water.	NA
O2	Molecular oxygen	mmol m^{-3}
NO3	Nitrate	mmol m^{-3}
NH4	Ammonium	mmol m^{-3}
PO4	Phosphate	mmol m^{-3}
Total_Phytoplankton	Total Phytoplankton	mmol m^{-3}
Primary_Production	Photosynthesis: Primary production	mmol m^{-2} d^{-1}
Water_Column_Respiration	Water column respiration	mmol m^{-2} d^{-1}
Air_Sea_O2_Flux	Air-Sea O2 flux	mmol m^{-2} d^{-1}
FPOM	Particulate Organic Matter Sediment-water Flux	mmol m^{-2} d^{-1}
FO2	O2 Sediment-water Flux	mmol m^{-2} d^{-1}
FNO3	NO3 Sediment-water Flux	mmol m^{-2} d^{-1}
FNH4	NH4 Sediment-water Flux	mmol m^{-2} d^{-1}
FPO4	PO4 Sediment-water Flux	mmol m^{-2} d^{-1}

4.2 WQEM

4.2.1 WQEM.000000.nc

Table 20. *WQEM.000000.nc file variables*

Variable Name	Description	Units
longitude	longitude	degrees
latitude	latitude	degrees
h	Cell bottom depth.	m
fm	Mask: 0 = land, 1 = water.	NA
dz	Thickness of cell.	NA
Area	Area of cell.	m^2
DOC	Dissolved organic Carbon.	kg m^{-3}
DIA	Diatom.	kg m^{-3}
GRE	Algae excluding diatoms.	kg m^{-3}
ZOO	Zooplankton.	kg m^{-3}
LOC	Labile particulate organic carbon.	kg m^{-3}
ROC	Refractory particulate organic carbon.	kg m^{-3}
SRP	Soluble reactive phosphorous.	kg m^{-3}
DOP	Dissolved organic phosphorous.	kg m^{-3}
LOP	Labile particulate organic phosphorous.	kg m^{-3}
ROP	Refractory particulate organic phosphorous.	kg m^{-3}
NH4	Ammonia.	kg m^{-3}
NO3	Nitrate plus nitrite nitrogen.	kg m^{-3}
DON	Dissolved organic nitrogen.	kg m^{-3}
LON	Labile particulate organic nitrogen.	kg m^{-3}
RON	Refractory particulate organic nitrogen.	kg m^{-3}
SA	Available silica.	kg m^{-3}
SU	Unavailable silica.	kg m^{-3}
DO2	Dissolved oxygen.	kg m^{-3}
TR	Tracer.	kg m^{-3}
DIAN	Diatoms Internal Nitrogen	kg m^{-3}
DIAP	Diatoms Internal Phosphorus	kg m^{-3}
GREN	Greens Internal Nitrogen	kg m^{-3}
GREP	Greens Internal Phosphorus	kg m^{-3}
SUM_DENITR	Denitrification N	kg m^{-3}
SUM_DENITR_C	Denitrification C	kg m^{-3}

Variable Name	Description	Units
SUM_DOCPRD	Carbon loss due to predation	kg m^{-3}
SUM_DOCMET	Carbon loss due to metabolism	kg m^{-3}
SUM_DOCZOO	Carbon loss due to zooplankton mortality	kg m^{-3}
PD	Production for diatoms	kg
PG	Production for greens	kg
NITDO2	Nitrification	kg
DOMETD	Diatoms respiration	kg
DOMETG	Greens respiration	kg
DOPREDD	Diatoms predation	kg
DOPREDG	Greens predation	kg
DOZOO	Zooplankton mortality	kg
DOMNLDOC	DOC mineralization	kg
PFD	Phosphorous limitation for diatoms	NA
SFD	Silica limitation for diatoms	NA
NFD	Nitrogen limitation for diatoms	NA
IFD	Light limitation for diatoms	NA
TFD	Temperature limitation for diatoms	NA
PFG	Phosphorous limitation for greens	NA
NFG	Nitrogen limitation for greens	NA
IFG	Light limitation for greens	NA
TFG	Temperature limitation for greens	NA
PAR	Photosynthetic Active Radiation	µmol quanta m^2 s^{-1}

5.0 Tutorials: Using CGEM

5.1 Overview

The following examples describe how to run simulations of varying dimensions (0, 1, 2, & 3D) and illustrates a small subset of the possible simulation options available. They are intended to assist new users with successfully running basic simulations, but do not attempt to encompass all possible model inputs, options, etc. available with CGEM.

More details on required input files for simulations are described in Section 3.1, "Required Input Files," on page 12. Sample submit scripts for the SLURM workload manager are available in the submitFiles directory.

5.2 0-D – Single Cell Example

5.2.1 Description

This example involves running a simulation with a single cell (0-D) grid. It allows for easy testing of the CGEM or WQEM water quality model without complications from advection, grid geometries, boundary conditions, etc. It also allows for the use of simple text-based inputs, as opposed to NetCDF formatted inputs required by higher dimensional simulations.

Files are supplied for multiple model settings, such as time-series temperature data (Temp.dat) or temperature data supplied by regression equation (T.dat). These settings can be controlled by editing the model input file (GEM_InputFIle_0D_example). For more details, refer to Section 3.2, "Input File Settings," on page 14.

5.2.2 Files Required

All files required for this example are available in the directory data/0D_example/:

- GEM_InputFile_0D_example – model input text file containing model specifications/switches. For more details, refer to Section 3.2, "Input File Settings," on page 14.
- InitialConditions.txt (or InitialConditions_WQEM.txt) – text file containing model initial conditions for the water quality model, CGEM (or WQEM)
- Model_dim.txt – text file containing model grid specifications
- S.dat - text file containing initialization value for salinity (if using Read_Sal = 0)
- T.dat - text file containing values for temperature regression equation (if using Read_T = 0)
- d.dat – text file containing depth value from surface to bottom of cell (only used in the 0-D model)
- d_sfc.dat – text file containing value for distance from cell center to surface
- dxdy.dat – text file containing values for cell length and width
- dz.dat – text file containing value for cell thickness in meters
- latlon.dat – text file containing value for cell latitude and longitude
- nz.dat – text file containing grid layout
- INPUT
  - Sal.dat – text file containing time-dependent salinity data (if using Read_Sal = 1)
  - Solar.dat – text file containing time-dependent solar radiation data (if using Read_Solar = 1)

- Temp.dat – text file containing time-dependent temperature data (if using Read_T = 1)
- Wind.dat – text file containing time-dependent wind data (if using Read_Wind = 1)

5.2.3 Running the simulation

1. Modify MyFiles.inp (located in the “data” directory) to provide a complete path to the 0D_example directory.

   Example:

   /work/GLFBREEZ/CGEM/data/0D_example

2. Modify InputFile (GEM_InputFile_0D_example) to set appropriate model settings. Rename the file to GEM_InputFile_0D.
3. Compile the serial CGEM executable using instructions in Section 2.3.1, "Serial Compilation," on page 10.
4. Start simulation (for more information, see Section 3.4, "Executable Command Line Arguments," on page 27) using a direct command line argument or batch script for a HPC workload manager.

   Example command line argument (from main CGEM directory containing “CGEM” executable):

   ./CGEM CGEM ./data/Examples/0D_example/GEM_InputFile_0D InitialConditions.txt ./NETCDF/0Dexample.

5.2.4 Viewing Results

Results will be written to a NetCDF file with filename and location as specified in the executable command line argument. For the example above, this file would be located at ./NETCDF/0Dexample.nc .

Use the R scripts found in Section 6.2, "R Scripts," on page 41 to visualize the 0-D results.

5.3 1-D – Vertical Column of Cells

5.3.1 Description

This example describes running a 1D simulation with a grid composed of a single column of cells. Like the 0D example, it allows for easy testing of the CGEM or WQEM water quality model without complications from advection, grid geometries, boundary conditions, etc, while also allowing multi-layer kinetics. It requires NetCDF formatted inputs similar to higher dimensional (2D & 3D) simulations.

Files are supplied for multiple model settings, such as time-series temperature data (Temp.dat) or temperature data supplied by regression equation (T.dat). These settings can be controlled by editing the model input file (GEM_InputFIle_0D_example). For more details, refer to Section 3.2, "Input File Settings," on page 14.

5.3.2 Files Required

- GEM_InputFile_1D_example - model input text file containing model specifications/switches. For more details, refer to Section 3.2, "Input File Settings," on page 14.

- InitialConditions.txt – text file containing model initial conditions for the water quality model (CGEM)
- Model_dim.txt – text file containing model grid specifications
- dxdy.dat – text file containing value for cell length and width
- latlon.dat – text file containing value for cell latitude and longitude
- REQUIRED INPUT (located in INPUT directory)
  - Solar.dat – text file containing time-dependent solar radiation data (if using Read_Solar = 1. For more details, refer to Section 3.2, "Input File Settings," on page 14.
  - Ev.nc – NetCDF file containing time-dependent diffusivity data
  - LayerDepth.nc – NetCDF file containing time-dependent layer depth data
  - Salt.nc – NetCDF file containing time-dependent salinity data
  - SurfaceElev.nc – NetCDF file containing time-dependent surface elevation data
  - Temp.nc – NetCDF file containing time-dependent temperature data
  - WaterDepth.nc – NetCDF file containing time-dependent water depth data
  - UFlow.nc – NetCDF file containing time-dependent velocity flux data for the x-direction
  - VFlow.nc – NetCDF file containing time-dependent velocity flux data for the y-direction
  - WFlow.nc – NetCDF file containing time-dependent velocity flux data for the z-direction

5.3.3 Running the simulation

1. Modify MyFiles.inp (located in the “data” directory) to provide a complete path to the 1D_example directory.

   Example:

   /work/GLFBREEZ/CGEM/data/1D_example

2. Modify InputFile (GEM_InputFile_1D_example) to set appropriate model settings and save it as GEM_InputFile_1D

3. Compile the serial CGEM executable using instructions in Section 2.3.1, "Serial Compilation," on page 10.

4. Start simulation (for more information, see Section 3.4, "Executable Command Line Arguments," on page 27) using a direct command line argument or batch script for a HPC workload manager.

   Example command line argument (from directory containing “CGEM” executable):

   ./CGEM CGEM ./data/Examples/1D_example/GEM_InputFile_1D InitialConditions.txt ./NETCDF/1Dexample.

5.3.4 Viewing Results

Results will be written to a NetCDF file with filename and location as specified in the executable command line argument. For the example above, this file would be located at ./NETCDF/1Dexample.nc .

Use the R scripts found in Section 6.2, "R Scripts," on page 41 to visualize these 1-D results.

5.4 2-D – Area of Cells (Single Layer)

5.4.1 Description

This example describes running a 2-D simulation involving an area of cells with single cell depth. This introduces complexity due to the use of advection and boundary conditions. This example is based on an EFDC hydrodynamic grid.

5.4.2 Files Required

- Depth.dat – text file containing depth specifications
- GEM_InputFile_2D_example - model input text file containing model specifications/switches (see Input File Settings)
- InitialConditions.txt – text file containing model initial conditions for the water quality model (CGEM)
- Model_dim.txt – text file containing model grid specifications
- dxdy.dat – text file containing value for cell length and width
- latlon.dat – text file containing value for cell latitude and longitude
- nz.dat – text file containing number of cells per water column
- REQUIRED INPUT (located in INPUT directory)
  - Solar.dat – text file containing time-dependent solar radiation data (if using Read_Solar = 1, see Input File Setting)
  - Ev.nc – NetCDF file containing time-dependent diffusivity data
  - LayerDepth.nc – NetCDF file containing time-dependent layer depth data
  - Salt.nc – NetCDF file containing time-dependent salinity data
  - SurfaceElev.nc – NetCDF file containing time-dependent surface elevation data
  - Temp.nc – NetCDF file containing time-dependent temperature data
  - WaterDepth.nc – NetCDF file containing time-dependent water depth data
  - UFlow.nc – NetCDF file containing time-dependent velocity flux data for the x-direction
  - VFlow.nc – NetCDF file containing time-dependent velocity flux data for the y-direction
  - WFlow.nc – NetCDF file containing time-dependent velocity flux data for the z-direction
- OPTIONAL INPUT (requires updates to Model_dim.txt)
  - Boundary Concentrations (optional for EFDC Hydro; to turn off boundary cells set “Number of boundary cells” (line 10) to 0 in Model_dim.txt)
    - BCindices.dat
    - /INPUT/TN_BoundaryConcentrations.nc
    - /INPUT/NO3_BoundaryConcentrations.nc
    - /INPUT/NH4_BoundaryConcentrations.nc
    - /INPUT/DON_BoundaryConcentrations.nc
    - /INPUT/TP_BoundaryConcentrations.nc
    - /INPUT/DIP_BoundaryConcentrations.nc
    - /INPUT/DOP_BoundaryConcentrations.nc
    - /INPUT/BOD_BoundaryConcentrations.nc
    - /INPUT/DO_BoundaryConcentrations.nc
  - River Loadings CGEM (optional for EFDC Hydro; to turn off river loading set “Number of rivers” (line 9) to 0 in Model_dim.txt)
    - RiverIndices.dat
    - RiverWeights.dat

- /INPUT/TN_RiverLoads.nc
- /INPUT/NO3_RiverLoads.nc
- /INPUT/NH3_RiverLoads.nc
- /INPUT/DON_RiverLoads.nc
- /INPUT/TP_RiverLoads.nc
- /INPUT/DIP_RiverLoads.nc
- /INPUT/DOP_RiverLoads.nc
- /INPUT/BOD1_RiverLoads.nc
- /INPUT/DO_RiverLoads.nc

- River Loadings WQEM (optional for EFDC Hydro)
  - /INPUT/TP_RiverLoads.nc
  - /INPUT/NO3_RiverLoads.nc
  - /INPUT/NH4_RiverLoads.nc
  - /INPUT/DON_RiverLoads.nc
  - /INPUT/DIP_RiverLoads.nc
  - /INPUT/DOP_RiverLoads.nc
  - /INPUT/DO_RiverLoads.nc

5.4.3 Running the simulation

1. Modify MyFiles.inp (located in the “data” directory) to provide complete path to the 2D_example directory.

   Example:

   /work/GLFBREEZ/CGEM/data/2D_example

2. Modify InputFile (GEM_InputFile_2D_example) to set appropriate model settings and save it as GEM_InputFile_2D

3. Compile the serial CGEM executable using instructions in Section 2.3.1, "Serial Compilation," on page 10.

4. Start simulation (for more information, see Section 3.4, "Executable Command Line Arguments," on page 27) using a direct command line argument or batch script for a HPC workload manager.

   Example sbatch script (for SLURM workload manager) “submit.sh” (placed in main CGEM directory containing “CGEM” executable):

   ```
   #!/bin/csh
   #SBATCH -J CGEM
   #SBATCH -t 4:00:00
   #SBATCH -N 2
   #SBATCH -n 32
   #SBATCH --gid=glfbreez
   #SBATCH -A glfbreez
   #SBATCH --partition=debug
   #SBATCH --output=logfile%j.log
   source modules_intel.sh
   mpirun ./CGEM CGEM ./data/Examples/2D_example/GEM_InputFile_2D
   InitialConditions.txt ./NETCDF/2Dexample.
   ```

   This sbatch script can be submitted to the SLURM workload manager with the command:

   ```
   sbatch submit.sh
   ```

The sbatch example script must be modified for use with a workload manager other than SLURM, such as PBS, LSF, etc.

5.4.4 Viewing Results

Results will be written to a NetCDF file with filename and location as specified in the executable command line argument. For the example above, this file would be located at ./NETCDF/2Dexample.nc .

Use the R scripts found in Section 6.2, "R Scripts," on page 41 to visualize these 2-D results.

5.5 3-D – Full 3-D Grid of Cells

5.5.1 Description

This example describes running a 3-D simulation involving an area of cells with multi-cell depth. This introduces complexity due to the use of advection and boundary conditions. This example is based on an EFDC hydrodynamic grid.

5.5.2 Files Required

- GEM_InputFile_3D_example - model input text file containing model specifications/switches. For more details, refer to Section 3.2, "Input File Settings," on page 14.
- InitialConditions.txt – text file containing model initial conditions for the water quality model (CGEM)
- Model_dim.txt – text file containing model grid specifications
- dxdy.dat – text file containing value for cell length and width
- latlon.dat – text file containing value for cell latitude and longitude
- nz.dat – text file containing number of cells per water column
- REQUIRED INPUT (located in INPUT directory)
  - Solar.dat – text file containing time-dependent solar radiation data (if using Read_Solar = 1, see Section 3.2, "Input File Settings," on page 14)
  - Ev.nc – NetCDF file containing time-dependent diffusivity data
  - LayerDepth.nc – NetCDF file containing time-dependent layer depth data
  - Salt.nc – NetCDF file containing time-dependent salinity data
  - SurfaceElev.nc – NetCDF file containing time-dependent surface elevation data
  - Temp.nc – NetCDF file containing time-dependent temperature data
  - WaterDepth.nc – NetCDF file containing time-dependent water depth data
  - UFlow.nc – NetCDF file containing time-dependent velocity flux data for the x-direction
  - VFlow.nc – NetCDF file containing time-dependent velocity flux data for the y-direction
  - WFlow.nc – NetCDF file containing time-dependent velocity flux data for the z-direction
- OPTIONAL INPUT (requires updates to Model_dim.txt)
  - Boundary Concentrations (optional for EFDC Hydro; to turn off boundary cells set “Number of boundary cells” (line 10) to 0 in Model_dim.txt))
    - BCindices.dat
    - /INPUT/TN_BoundaryConcentrations.nc
    - /INPUT/NO3_BoundaryConcentrations.nc

- /INPUT/NH4_BoundaryConcentrations.nc
- /INPUT/DON_BoundaryConcentrations.nc
- /INPUT/TP_BoundaryConcentrations.nc
- /INPUT/DIP_BoundaryConcentrations.nc
- /INPUT/DOP_BoundaryConcentrations.nc
- /INPUT/BOD_BoundaryConcentrations.nc
- /INPUT/DO_BoundaryConcentrations.nc

- River Loadings CGEM (optional for EFDC Hydro; to turn off river loading set "Number of rivers" (line 9) to 0 in Model_dim.txt)
  - RiverIndices.dat
  - RiverWeights.dat
  - /INPUT/TN_RiverLoads.nc
  - /INPUT/NO3_RiverLoads.nc
  - /INPUT/NH3_RiverLoads.nc
  - /INPUT/DON_RiverLoads.nc
  - /INPUT/TP_RiverLoads.nc
  - /INPUT/DIP_RiverLoads.nc
  - /INPUT/DOP_RiverLoads.nc
  - /INPUT/BOD1_RiverLoads.nc
  - /INPUT/DO_RiverLoads.nc
- River Loadings WQEM (optional for EFDC Hydro)
  - /INPUT/TP_RiverLoads.nc
  - /INPUT/NO3_RiverLoads.nc
  - /INPUT/NH4_RiverLoads.nc
  - /INPUT/DON_RiverLoads.nc
  - /INPUT/DIP_RiverLoads.nc
  - /INPUT/DOP_RiverLoads.nc
  - /INPUT/DO_RiverLoads.nc

5.5.3 Running the simulation

1. Modify MyFiles.inp (located in the "data" directory) to provide complete path to the 3D_example directory.

   Example:

   /work/GLFBREEZ/CGEM/data/3D_example

2. Modify InputFile (GEM_InputFile_3D_example) to set appropriate model settings and save it as GEM_InputFile_3D
3. Compile the serial CGEM executable using instructions in Section 2.3.1, "Serial Compilation," on page 10.
4. Start simulation (for more information, see Section 3.4, "Executable Command Line Arguments," on page 27) using a direct command line argument or batch script for a HPC workload manager.

   Example sbatch script (for SLURM workload manager) "submit.sh" (placed in main CGEM directory containing "CGEM" executable):

```
#!/bin/csh
#SBATCH -J CGEM
#SBATCH -t 4:00:00
#SBATCH -N 2
#SBATCH -n 32
#SBATCH --gid=glfbreez
```

```
#SBATCH -A glfbreez
#SBATCH --partition=debug
#SBATCH --output=logfile%j.log
source modules_intel.sh
mpirun ./CGEM CGEM ./data/Examples/3D_example/GEM_InputFile_3D
InitialConditions.txt ./NETCDF/3Dexample.
```

This sbatch script can be submitted to the SLURM workload manager with the command:

```
sbatch submit.sh
```

The sbatch example script must be modified for use with a workload manager other than SLURM, such as PBS, LSF, etc.

5.5.4 Viewing Results

Results will be written to a NetCDF file with filename and location as specified in the executable command line argument. For the example above, this file would be located at ./NETCDF/3Dexample.nc .

Use the R scripts found in Section 6.2, "R Scripts," on page 41 to visualize these 3-D results.

6.0 Other Scripts and Utilities

6.1 EFDC Utility

Coupling of the Environmental Fluid Dynamics Code (EFDC) with CGEM/WQEM is facilitated by a standalone utility developed to post-process a hydrodynamic output file from EFDC, labeled with the suffix ".hyd." This utility converts binary model output from the .hyd file into netcdf formats required by CGEM/WQEM for advection and mixing in 1-D, 2-D, and 3-D models. Detailed instructions for the compilation and application of the EFDC utility is provided in the EFDC Utility User Guide.

6.2 R Scripts

Several R scripts are included with the distribution of the CGEM source code. These R scripts perform various tasks such as generating timeseries plots of state variable concentrations, mass balance checks, and state variable comparisons, among others. All R scripts listed below assume the default names of the CGEM and WQEM outputs are cgem.000000.nc and wqem.000000.nc, respectively. These default names can be changed to some other name within the scripts. Before attempting to run any of these scripts, place copies of them on the same directory where the model output is. The general command to run any of these scripts on the command line is:

Rscript <name_of_script> <model>

where

<name_of_script> = name of script including the "R" extension

<model> = cgem or wqem

The R scripts can be grouped by the number of dimensions used in the CGEM run: 0D, 1D, and 3D.

6.2.1 0-D Scripts

- make_plots_0D.R - This script makes plots for the 0D models. To run this script enter "Rscript make_plots_0D.R cgem" or "Rscript make_plots_0D.R wqem" at the command-line prompt. It uses the scripts below.
  - allvars_0D.R - This script loops over every state variable and generates timeseries plots. It uses the following script:
    - timeseries_plot.R - This script generates a timeseries plot.

6.2.2 1-D Scripts

- make_plots_1D.R - This is the main script for plotting a timeseries of every variable in the output of the 1D model. To run this script enter "Rscript make_plots_1D.R cgem" or "Rscript make_plots_1D.R wqem" at the command-line prompt. This script uses the following scripts:
  - allvars_1D.R - This script loops over every variable and calls functions contained in the script below. The indices of the vertical layers must be set inside the script.
    - timeseries_plot.R - This script generates a timeseries plot.
  - allvars_1D_depth.R - This script plots depth profiles at selected days. The days must be set inside the script.

- make_plots_1D_EFDC.R - This is the main script for plotting timeseries of every state variable in the output of the EFDC-1D model for selected vertical layers. This script is similar to “make_plots_1D.R” except it handles EFDC output.

  To run the script enter "Rscript make_plots_1D_EFDC.R cgem" or "Rscript make_plots_1D_EFDC.R wqem" at the command-line prompt. This script uses the scripts below.

- allvars_1D_EFDC.R - This script loops over every variable and calls functions contained in the script below. The indices of the vertical layers must be set inside this script.
  - timeseries_plot.R - This script generates a timeseries plot.
- allvars_1D_separate.R - This script is similar to “allvars_1D.R” except that it processes separate timeseries plots (as opposed to putting multiple plots in the same page). This script is meant to be called by “make_plots_1D.R”. It calls the functions contained in the script below.
  - timeseries_plot.R - This script generates a timeseries plot.
- massTR_1D.R - This script calculates the percent difference of the Tracer concentration with respect to its initial value for each timestep, plots the results, and stores the plots in a PDF file. It can only be run for the 1D model.

6.2.3 2-D & 3-D Scripts

- make_plots_3D_EFDC.R - This is the main script for plotting a timeseries of every state variable in the output of the EFDC-3D model for selected vertical layers. This script is similar to “make_plots_1D_EFDC.R”. To run the script enter "Rscript make_plots_3D_EFDC.R cgem" or "Rscript make_plots_3D_EFDC.R wqem" at the command-line prompt. It uses the scripts below.
  - allvars_3D_EFDC.R - This script loops over every state variable and calls the script below to generate timeseries plots. The indices of the vertical layers must be set inside the script.
    - timeseries_plot.R - This script generates a timeseries plot.
  - massTR.R - This script calculates the percent difference of the Tracer concentration with respect to its initial value for each timestep, plots the results, and stores the plots in a PDF file. It is set up to be used for the 3D model. The dimensions of the grid must be set inside the script.

6.2.4 Mass Balance Scripts

- MB_C.R - This script calculates the total carbon in the system as a function of time and stores the results in a text file. This script only works for CGEM output. The script is currently set up for the 1D model with six phytoplankton classes although it can be easily generalized to the 3D case. To run the script enter “Rscript MB_C.R” at the command-line prompt.
- MB_N.R - This script calculates the total nitrogen in the system as a function of time and stores the results in a text file. This script only works for CGEM output. The script is currently set up for the 1D model with six phytoplankton classes although it can be easily generalized to the 3D case. To run the script enter “Rscript MB_N.R” at the command-line prompt.
- MB_PO4.R - This script calculates the total phosphate in the system as a function of time and stores the results in a text file. This script only works for CGEM output. The script is currently set up for the 1D model with six

phytoplankton classes although it can be easily generalized to the 3D case. To run the script enter “Rscript MB_PO4.R” at the command-line prompt.

7.0 References

Beck, M., Lehrter, J.C., Lowe, L.L., Jarvis, B.M. (2018). Parameter sensitivity and identifiability for a biogeochemical model of hypoxia in the northern Gulf of Mexico. Ecol Modell. 2017 Nov 10; 363: 17–30.

Cerco, C. and T. Cole. 1995. User's Guide to the CE-QUAL-ICM Three-Dimensional Eutrophication Model. U.S. Army Corps of Engineers, U.S. Army Engineer Waterways Experiment Station, Vicksburg, Mississippi. Technical Report EL-95-15, 2,420 pp.

Eldridge, P. M., and Roelke, D. L.: Origins and scales of hypoxia on the Louisiana shelf: Importance of seasonal plankton dynamics and river nutrients and discharge, Ecological Modelling, 221, 1028-1042, http://dx.doi.org/10.1016/j.ecolmodel.2009.04.054, 2010.

Feist, T.J., Pauer, J.J., Melendez, W. Lehrter, J.C., DePetro, P.A., Rygwelski, K.R., Ko, D.S., Kreis, R.G. Jr. 2016. Modeling the Relative Importance of Nutrient and Carbon Loads, Boundary Fluxes, and Sediment Fluxes on Gulf of Mexico Hypoxia. Environ. Sci. Technol. 50, 8713-8721

Jarvis, Brandon and Hagy, James D. and Melendez, Wilson and Simmons, Cody W. and Wan, Yongshan, Measuring and Modeling Diel Oxygen Dynamics in a Shallow Hypereutrophic Estuary: Implications of Low Oxygen Exposure on Aquatic Life. http://dx.doi.org/10.2139/ssrn.4333571

Jarvis B, Greene RM, Wan Y, Lehrter JC, Lowe LL, Ko DS (2021) Contiguous Low Oxygen Waters between the Continental Shelf Hypoxia Zone and Nearshore Coastal Waters of Louisiana, USA: Interpreting 30 Years of Profiling Data and Three-Dimensional Ecosystem Modeling. Environ. Sci. Technol. https://dx.doi.org/10.1021/acs.est.0c05973

Jarvis, B., Pauer, J., Melendez, W., Simmons, C., Wan, Y. et al. (2021) Inter-model comparison of simulated Gulf of Mexico hypoxia in response to reduced nutrient loads: Effects of phytoplankton and organic matter parameterization. Environmental Modelling & Software. https://doi.org/10.1016/j.envsoft.2022.105365

Jarvis B., Lehrter, J., Lowe, L., Hagy, J., Wan, Y., Murrell, M., Ko, D., Penta, B., Gould, R. (2020). Modeling Spatiotemporal Patterns of Ecosystem Metabolism and Organic Carbon Dynamics Affecting Hypoxia on the Louisiana Continental Shelf. JGR-Oceans. https://doi.org/10.1029/2019JC015630

Lehrter JC, Ko DS, Lowe L, Penta B. 2017. Predicted Effects of Climate Change on Northern Gulf of Mexico Hypoxia. Chapter 8 in: Justic et al. (eds.). Modeling Coastal Hypoxia: Numerical simulations of Patterns, Controls, and Effect of Dissolved Oxygen Dynamics. Springer, New York.

Pauer, J., W. Melendez, T. Feist, J. Lehrter, B. Rashleigh, L. Lowe, and R. Greene (2020). “The impact of an alternative model structure and computational grid size on model predicted primary production and hypoxic area in the northern Gulf of Mexico”. Environmental Modelling and Software. https://doi.org/10.1016/j.envsoft.2020.104661

Pauer, J., Rowe, M.D., Melendez, W., Robertson, D., Alsip, P., Lowe, L., and Hollenhorst, T. A (2022). modeling study to describe and predict nearshore phosphorus concentrations in Lake Michigan. Journal of Great Lakes Research. 48, 2. 343-358. https://doi.org/10.1016/j.jglr.2021.09.014

Pauer, J.J., Feist, T.J., Anstead, A.M., DePetro, P.A., Melendez, W., Lehrter, J.C., Murrell, M.C., Zhang, X., Ko, D.S., 2016. A modeling study examining the impact of nutrient boundaries on primary production on the Louisiana continental shelf. Ecol Modell 328, 136−147.

Appendix A:NetCDF Input File Metadata

A.1 Hydrodynamic Data

A.1.1 U Flows

```
netcdf UFlow {
dimensions:
    X = 24 ;
    Y = 24;
    Z = 4 ;
    Time = 2881 ;
variables:
    int X(X) ;
        X:units = "meters" ;
        X:long_name = "X" ;
    int Y(Y) ;
        Y:units = "meters" ;
        Y:long_name = "Y" ;
    int Z(Z) ;
        Z:units = "meters" ;
        Z:long_name = "Z" ;
    double Time(Time) ;
        Time:units = "seconds" ;
        Time:long_name = "Time" ;
    float UFlow(Time, Z, Y, X) ;
        UFlow:units = "m3/s" ;
        UFlow:_FillValue = -9999.f ;
}
```

A.1.2 V Flows

```
netcdf VFlow {
dimensions:
    X = 24 ;
    Y = 24 ;
    Z = 4 ;
    Time = 2881 ;
```

variables:

int X(X) ;

X:units = "meters" ;

X:long_name = "X" ;

int Y(Y) ;

Y:units = "meters" ;

Y:long_name = "Y" ;

int Z(Z) ;

Z:units = "meters" ;

Z:long_name = "Z" ;

double Time(Time) ;

Time:units = "seconds" ;

Time:long_name = "Time" ;

float VFlow(Time, Z, Y, X) ;

VFlow:units = "m3/s" ;

VFlow:_FillValue = -9999.f ;

}

A.1.3 W Flows

netcdf WFlow {

dimensions:

X = 24 ;

Y = 24 ;

Z = 4 ;

Time = 2881 ;

variables:

int X(X) ;

X:units = "meters" ;

X:long_name = "X" ;

int Y(Y) ;

Y:units = "meters" ;

Y:long_name = "Y" ;

int Z(Z) ;

Z:units = "meters" ;

Z:long_name = "Z" ;

double Time(Time) ;

Time:units = "seconds" ;

Time:long_name = "Time" ;

float WFlow(Time, Z, Y, X) ;

WFlow:units = "m3/s" ;

WFlow:_FillValue = -9999.f ;

}

A.1.4 Vertical Mixing Coefficients

netcdf Ev {

dimensions:

X = 24 ;

Y = 24 ;

Z = 4 ;

Time = 2881 ;

variables:

int X(X) ;

X:units = "meters" ;

X:long_name = "X" ;

int Y(Y) ;

Y:units = "meters" ;

Y:long_name = "Y" ;

int Z(Z) ;

Z:units = "meters" ;

Z:long_name = "Z" ;

double Time(Time) ;

Time:units = "seconds" ;

Time:long_name = "Time" ;

float Ev(Time, Z, Y, X) ;

Ev:units = "m2/s" ;

:_FillValue = -9999.f ;

}

A.1.5 Surface Elevation

netcdf SurfaceElev {

dimensions:

X = 24 ;

Y = 24 ;

```
        Time = 2881 ;
    variables:
        int X(X) ;
            X:units = "meters" ;
            X:long_name = "X" ;
        int Y(Y) ;
            Y:units = "meters" ;
            Y:long_name = "Y" ;
        int Z(Time) ;
            Z:units = "meters" ;
            Z:long_name = "Z" ;
        double Time(Time) ;
            Time:units = "seconds" ;
            Time:long_name = "Time" ;
        float SurfaceElev(Time, Y, X) ;
            SurfaceElev:units = "meters" ;
            SurfaceElev:_FillValue = -9999.f ;
    }
```

A.1.6 Volume

```
    netcdf Volume {
    dimensions:
        X = 24 ;
        Y = 24 ;
        Z = 4 ;
        Time = 2881 ;
    variables:
        int X(X) ;
            X:units = "meters" ;
            X:long_name = "X" ;
        int Y(Y) ;
            Y:units = "meters" ;
            Y:long_name = "Y" ;
        int Z(Z) ;
            Z:units = "meters" ;
            Z:long_name = "Z" ;
        double Time(Time) ;
```

```
        Time:units = "seconds" ;
        Time:long_name = "Time" ;
    float Volume(Time, Z, Y, X) ;
        Volume:units = "m3" ;
        Volume:_FillValue = -9999.f ;
}
```

A.1.7 Water Depth

```
netcdf WaterDepth {
dimensions:
    X = 24 ;
    Y = 24 ;
    Time = 2881 ;
variables:
    int X(X) ;
        X:units = "meters" ;
        X:long_name = "X" ;
    int Y(Y) ;
        Y:units = "meters" ;
        Y:long_name = "Y" ;
    int Z(Time) ;
        Z:units = "meters" ;
        Z:long_name = "Z" ;
    double Time(Time) ;
        Time:units = "seconds" ;
        Time:long_name = "Time" ;
    float WaterDepth(Time, Y, X) ;
        WaterDepth:units = "meters" ;
        WaterDepth:_FillValue = -9999.f ;
}
```

A.1.8 Layer Depth

```
netcdf LayerDepth {
dimensions:
    X = 24 ;
    Y = 24 ;
```

```
        Z = 4 ;
        Time = 2881 ;
    variables:
        int X(X) ;
            X:units = "meters" ;
            X:long_name = "X" ;
        int Y(Y) ;
            Y:units = "meters" ;
            Y:long_name = "Y" ;
        int Z(Z) ;
            Z:units = "meters" ;
            Z:long_name = "Z" ;
        double Time(Time) ;
            Time:units = "seconds" ;
            Time:long_name = "Time" ;
        float LayerDepth(Time, Z, Y, X) ;
            LayerDepth:units = "meters" ;
            LayerDepth:_FillValue = -9999.f ;
    }
```

A.1.9 Temperature

```
    netcdf Temp {
    dimensions:
        X = 24 ;
        Y = 24 ;
        Z = 4 ;
        Time = 2881 ;
    variables:
        int X(X) ;
            X:units = "meters" ;
            X:long_name = "X" ;
        int Y(Y) ;
            Y:units = "meters" ;
            Y:long_name = "Y" ;
        int Z(Z) ;
            Z:units = "meters" ;
            Z:long_name = "Z" ;
```

```
        double Time(Time) ;
            Time:units = "seconds" ;
            Time:long_name = "Time" ;
        float Temp(Time, Z, Y, X) ;
            Temp:units = "Celsius" ;
            Temp:_FillValue = -9999.f ;
}
```

A.1.10 Salinity

```
netcdf Salt {
dimensions:
        X = 24 ;
        Y = 24 ;
        Z = 4 ;
        Time = 2881 ;
variables:
        int X(X) ;
            X:units = "meters" ;
            X:long_name = "X" ;
        int Y(Y) ;
            Y:units = "meters" ;
            Y:long_name = "Y" ;
        int Z(Z) ;
            Z:units = "meters" ;
            Z:long_name = "Z" ;
        double Time(Time) ;
            Time:units = "seconds" ;
            Time:long_name = "Time" ;
        float Salt(Time, Z, Y, X) ;
            Salt:units = "ppt" ;
            Salt:_FillValue = -9999.f ;
}
```

A.2 River Loads

The current CGEM model can input river loads for 9 state variables: BOD1, DIP, DON, DOP, DO, NH3, NO3, TN, and TP. The current WQEM model can input river loads for 7 state variables: DIP, DON, DOP, DO, NH3, NO3, and TP.

Each state variable has its own netcdf file containing its river loads. The format of these files is the same for all state variables. An example of this format is:

netcdf <State_Variable>_RiverLoads {

dimensions:

Number_Rivers = 8 ;

Time = 304 ;

variables:

int Number_Rivers(Number_Rivers) ;

Number_Rivers:units = "unitless" ;

Number_Rivers:long_name = "Number_Rivers" ;

double Time(Time) ;

Time:units = "seconds" ;

Time:long_name = "Time" ;

float <State_Variable>(Time, Number_Rivers) ;

<State_Variable>:units = "kg/s" ;

}

where <State_Variable> = BOD1, DIP, DON, DOP, DO, NH3, NO3, TN, or TP.

A.3 Boundary Conditions

The current CGEM model can input boundary concentrations for 9 state variables: BOD, DIP, DON, DOP, DO, NH3, NO3, TN, and TP. The current WQEM model can input boundary concentrations for seven state variables: DIP, DON, DOP, DO, NH3, NO3, and TP.

Each state variable has its own netcdf file containing its boundary concentrations. The format of these files is the same for all state variables. An example of this format is:

netcdf <State_Variable>_BoundaryConcentrations {

dimensions:

Number_BoundaryCells = 12 ;

Time = 2 ;

variables:

int Number_BoundaryCells(Number_BoundaryCells) ;

Number_BoundaryCells:units = "unitless" ;

Number_BoundaryCells:long_name = "Number_BoundaryCells" ;

double Time(Time) ;

Time:units = "seconds" ;

Time:long_name = "Time" ;

float <State_Variable> (Time, Number_BoundaryCells) ;

<State_Variable>:units = "mg/l" ;

}

where <State_Variable> = BOD, DIP, DON, DOP, DO, NH3, NO3, TN, or TP.

Appendix B: CGEM Directory Structure

```
|-- CGEM
|   |-- GEM_InputFile
|   |-- GEM_InputFile_save
|   |-- Makefile
|   |-- Makefile_par_gen
|   |-- Makefile_serial_gen
|   |-- NETCDF
|   |   |-- AllVars_GoMDOM.R
|   |   |-- MB_C.R
|   |   |-- MB_N.R
|   |   |-- MB_PO4.R
|   |   |-- MultiVarPng.R
|   |   |-- R3D_timeseries.R
|   |   |-- allvars_0D.R
|   |   |-- allvars_1D.R
|   |   |-- allvars_1D_EFDC.R
|   |   |-- allvars_1D_depth.R
|   |   |-- allvars_1D_separate.R
|   |   |-- allvars_3D_EFDC.R
|   |   |-- compare_vars_1D.R
|   |   |-- compare_vars_1D_4.R
|   |   |-- compare_vars_1D_4_all.R
|   |   |-- compare_vars_depth.R
|   |   |-- compare_vars_depth7.R
|   |   |-- compare_vars_sub_1D.R
|   |   |-- debug.R
|   |   |-- make_plots_0D.R
|   |   |-- make_plots_1D.R
|   |   |-- make_plots_1D_EFDC.R
|   |   |-- make_plots_1D_compare.R
|   |   |-- make_plots_1D_compare4.R
|   |   |-- make_plots_1D_compare7.R
|   |   |-- make_plots_3D_EFDC.R
|   |   |-- massTR.R
|   |   |-- massTR_1D.R
```

```
|   |   `-- timeseries_plot.R
|   |-- SDM
|   |   |-- hypox_input.csv
|   |   |-- normoxia.dat
|   |   `-- ph2bprofile.dat
|   |-- WQEM_InputFile
|   |-- WQEM_InputFile_LakeOntario
|   |-- WQEM_InputFile_save
|   |-- cgem_src
|   |   |-- Allocate_Input_CGEM.F90
|   |   |-- CGEM.F90
|   |   |-- CGEM_Flux.F90
|   |   |-- CGEM_vars.F90
|   |   |-- Calc_Chla.F90
|   |   |-- Call_IOP_PAR.F90
|   |   |-- Check_InputFile_CGEM.F90
|   |   |-- DailyRad.F90
|   |   |-- DailyRad_init.F90
|   |   |-- Flux_CGEM.F90
|   |   |-- INPUT_VARS_CGEM.F90
|   |   |-- InitError_Check_CGEM.F90
|   |   |-- Init_Output_CGEM.F90
|   |   |-- JWMod.F90
|   |   |-- JW_SOC.F90
|   |   |-- Light_WQEM.F90
|   |   |-- MASS_BALANCE_CGEM.F90
|   |   |-- MATLAB.F90
|   |   |-- MC_Flux.F90
|   |   |-- MC_GEM.F90
|   |   |-- Meta_SOC.F90
|   |   |-- Mod_Filedata2.F90
|   |   |-- Model_Compare.F90
|   |   |-- Model_Diagenesis.F90
|   |   |-- Model_Finalize_CGEM.F90
|   |   |-- Model_Output_CGEM.F90
|   |   |-- OUTPUT_NETCDF_CGEM.F90
|   |   |-- OUTPUT_NOTCLOERN.F90
```

```
|  |  |-- OUTPUT_NRL.F90
|  |  |-- Read_InputFile_CGEM.F90
|  |  |-- SDM.F90
|  |  |-- STOICH_VARS.F90
|  |  |-- Salinity_Regression_Init_CGEM.F90
|  |  |-- Sediment_Diagenesis_Flux.F90
|  |  |-- Sediment_Diagenesis_Routines.F90
|  |  |-- Set_Initial_Conditions_CGEM.F90
|  |  |-- T_WQEM.F90
|  |  |-- Transport_CGEM.F90
|  |  |-- Write_InputFile_CGEM.F90
|  |  |-- calc_Agrow.F90
|  |  |-- changeA.F90
|  |  |-- func_E.F90
|  |  |-- func_Qs.F90
|  |  |-- func_S.F90
|  |  |-- func_T.F90
|  |  |-- nparray.F90
|  |  `-- src_files
|  |-- data
|  |  |-- Examples
|  |  |  |-- 0D_example
|  |  |  |  |-- GEM_InputFile_0D_example
|  |  |  |  |-- INPUT
|  |  |  |  |  |-- Sal.dat
|  |  |  |  |  |-- Solar.dat
|  |  |  |  |  |-- Temp.dat
|  |  |  |  |  `-- Wind.dat
|  |  |  |  |-- InitialConditions.txt
|  |  |  |  |-- InitialConditions_GD.txt
|  |  |  |  |-- Model_dim.txt
|  |  |  |  |-- S.dat
|  |  |  |  |-- T.dat
|  |  |  |  |-- Vol.dat
|  |  |  |  |-- d.dat
|  |  |  |  |-- d_sfc.dat
|  |  |  |  |-- dxdy.dat
```

```
|  |  |  |  |-- dz.dat
|  |  |  |  |-- latlon.dat
|  |  |  |  `-- nz.dat
|  |  |  |-- 1D_example
|  |  |  |  |-- Depth.dat
|  |  |  |  |-- GEM_InputFile_1D_example
|  |  |  |  |-- INPUT
|  |  |  |  |  |-- E.nc
|  |  |  |  |  |-- Ev.nc
|  |  |  |  |  |-- KH.nc
|  |  |  |  |  |-- LayerDepth.nc
|  |  |  |  |  |-- S.nc
|  |  |  |  |  |-- Salt.nc
|  |  |  |  |  |-- Solar.dat
|  |  |  |  |  |-- SurfaceElev.nc
|  |  |  |  |  |-- T.nc
|  |  |  |  |  |-- Temp.nc
|  |  |  |  |  |-- U.nc
|  |  |  |  |  |-- UFlow.nc
|  |  |  |  |  |-- V.nc
|  |  |  |  |  |-- VFlow.nc
|  |  |  |  |  |-- W.nc
|  |  |  |  |  |-- WFlow.nc
|  |  |  |  |  `-- WaterDepth.nc
|  |  |  |  |-- InitialConditions.txt
|  |  |  |  |-- InitialConditions_WQEM.txt
|  |  |  |  |-- Model_dim.txt
|  |  |  |  |-- TopoS.dat
|  |  |  |  |-- d.dat
|  |  |  |  |-- dxdy.dat
|  |  |  |  |-- latlon.dat
|  |  |  |  |-- lxly.dat
|  |  |  |  |-- mask.dat
|  |  |  |  `-- nz.dat
|  |  |  |-- 2D_example
|  |  |  |  |-- GEM_InputFile_2d_example
|  |  |  |  |-- INPUT
```

```
|  |  |  |  |  |-- BOD1_RiverLoads.nc
|  |  |  |  |  |-- BOD_BoundaryConcentrations.nc
|  |  |  |  |  |-- DIP_BoundaryConcentrations.nc
|  |  |  |  |  |-- DIP_RiverLoads.nc
|  |  |  |  |  |-- DON_BoundaryConcentrations.nc
|  |  |  |  |  |-- DON_RiverLoads.nc
|  |  |  |  |  |-- DOP_BoundaryConcentrations.nc
|  |  |  |  |  |-- DOP_RiverLoads.nc
|  |  |  |  |  |-- DO_BoundaryConcentrations.nc
|  |  |  |  |  |-- DO_RiverLoads.nc
|  |  |  |  |  |-- Ev.nc
|  |  |  |  |  |-- LayerDepth.nc
|  |  |  |  |  |-- NH3_RiverLoads.nc
|  |  |  |  |  |-- NH4_BoundaryConcentrations.nc
|  |  |  |  |  |-- NO3_BoundaryConcentrations.nc
|  |  |  |  |  |-- NO3_RiverLoads.nc
|  |  |  |  |  |-- Salt.nc
|  |  |  |  |  |-- Solar.dat
|  |  |  |  |  |-- SurfaceElev.nc
|  |  |  |  |  |-- TN_BoundaryConcentrations.nc
|  |  |  |  |  |-- TN_RiverLoads.nc
|  |  |  |  |  |-- TP_BoundaryConcentrations.nc
|  |  |  |  |  |-- TP_RiverLoads.nc
|  |  |  |  |  |-- Temp.nc
|  |  |  |  |  |-- UFlow.nc
|  |  |  |  |  |-- VFlow.nc
|  |  |  |  |  |-- Volume.nc
|  |  |  |  |  |-- WFlow.nc
|  |  |  |  |  `-- WaterDepth.nc
|  |  |  |  |-- InitialConditions.txt
|  |  |  |  |-- InitialConditions_WQEM.txt
|  |  |  |  |-- Model_dim.txt
|  |  |  |  |-- WQEM_InputFile_2D_example
|  |  |  |  |-- cell.inp
|  |  |  |  |-- control.dat
|  |  |  |  |-- d.dat
|  |  |  |  |-- dxdy.dat
```

```
|  |  |  |  |-- dxdy.inp
|  |  |  |  |-- latlon.dat
|  |  |  |  |-- lxly.dat
|  |  |  |  |-- lxly.inp
|  |  |  |  `-- nz.dat
|  |  |  |-- 3D_example
|  |  |  |  |-- GEM_InputFile_3d_example
|  |  |  |  |-- INPUT
|  |  |  |  |  |-- BOD1_RiverLoads.nc
|  |  |  |  |  |-- BOD_BoundaryConcentrations.nc
|  |  |  |  |  |-- DIP_BoundaryConcentrations.nc
|  |  |  |  |  |-- DIP_RiverLoads.nc
|  |  |  |  |  |-- DON_BoundaryConcentrations.nc
|  |  |  |  |  |-- DON_RiverLoads.nc
|  |  |  |  |  |-- DOP_BoundaryConcentrations.nc
|  |  |  |  |  |-- DOP_RiverLoads.nc
|  |  |  |  |  |-- DO_BoundaryConcentrations.nc
|  |  |  |  |  |-- DO_RiverLoads.nc
|  |  |  |  |  |-- Ev.nc
|  |  |  |  |  |-- LayerDepth.nc
|  |  |  |  |  |-- NH3_RiverLoads.nc
|  |  |  |  |  |-- NH4_BoundaryConcentrations.nc
|  |  |  |  |  |-- NO3_BoundaryConcentrations.nc
|  |  |  |  |  |-- NO3_RiverLoads.nc
|  |  |  |  |  |-- Salt.nc
|  |  |  |  |  |-- Solar.dat
|  |  |  |  |  |-- SurfaceElev.nc
|  |  |  |  |  |-- TN_BoundaryConcentrations.nc
|  |  |  |  |  |-- TN_RiverLoads.nc
|  |  |  |  |  |-- TP_BoundaryConcentrations.nc
|  |  |  |  |  |-- TP_RiverLoads.nc
|  |  |  |  |  |-- Temp.nc
|  |  |  |  |  |-- UFlow.nc
|  |  |  |  |  |-- VFlow.nc
|  |  |  |  |  |-- Volume.nc
|  |  |  |  |  |-- WFlow.nc
|  |  |  |  |  `-- WaterDepth.nc
```

```
|  |  |  |  |-- InitialConditions.txt
|  |  |  |  |-- InitialConditions_WQEM.txt
|  |  |  |  |-- Model_dim.txt
|  |  |  |  |-- WQEM_InputFile_3D_example
|  |  |  |  |-- d.dat
|  |  |  |  |-- dxdy.dat
|  |  |  |  |-- latlon.dat
|  |  |  |  |-- lxly.dat
|  |  |  |  `-- nz.dat
|  |  |-- MyFiles.inp
|  |  `-- MyFiles.inp_save
|  |-- main_src
|  |  |-- Adv3D.F90
|  |  |-- AdvNeighborsOrdered.F90
|  |  |-- AdvNeighborsOrdered_fake.F90
|  |  |-- Allocate_Input_Vars.F90
|  |  |-- Ave_istep_Offset.F90
|  |  |-- BoundaryConcentration.F90
|  |  |-- Calc_Sal.F90
|  |  |-- Calc_Temp.F90
|  |  |-- Command_Line_Args.F90
|  |  |-- Conversions.F90
|  |  |-- DATE_TIME.F90
|  |  |-- Decomp1D.F90
|  |  |-- Flux.F90
|  |  |-- Get_Vars.F90
|  |  |-- Grid.F90
|  |  |-- Hydro.F90
|  |  |-- INPUT_VARS.F90
|  |  |-- Initialize_Output.F90
|  |  |-- Initialize_State_Vars.F90
|  |  |-- Interp_utils.F90
|  |  |-- JY.F90
|  |  |-- LIGHT_VARS.F90
|  |  |-- MOD_UTILITIES.F90
|  |  |-- MPI_dummy.F90
|  |  |-- Model_Finalize.F90
```

| | |-- Model_Output.F90
| | |-- Model_dim.F90
| | |-- NETCDF_UTILITIES.F90
| | |-- Nitrification.F90
| | |-- OUTPUT.F90
| | |-- OUTPUT_ALL_FALSE.F90
| | |-- PNETCDF_UTILITIES.F90
| | |-- Q10_T.F90
| | |-- Read_CMAQ_NH4_SVflux_bin.F90
| | |-- Read_CMAQ_NO3_SVflux_bin.F90
| | |-- Read_InputFile.F90
| | |-- RiverLoad.F90
| | |-- State_Vars.F90
| | |-- TEMP_VARS.F90
| | |-- Transport.F90
| | |-- USER_Read_Sal.F90
| | |-- USER_Read_Solar.F90
| | |-- USER_Read_Temp.F90
| | |-- USER_Read_Wind.F90
| | |-- USER_Set_Initial_Conditions.F90
| | |-- USER_getLonLat.F90
| | |-- USER_get_EFDC_grid.F90
| | |-- USER_get_NCOM_grid.F90
| | |-- USER_get_POM_grid.F90
| | |-- USER_get_basic_grid.F90
| | |-- USER_get_masks.F90
| | |-- VMixing.F90
| | |-- WQ_Model.F90
| | |-- Which_Flux.F90
| | |-- blah
| | |-- calc_solar_zenith.F90
| | |-- error.F90
| | |-- fake_mpi_interface.F90
| | |-- fillval.F90
| | |-- getSolar.F90
| | |-- main.F90
| | |-- mpi_interface.F90

```
|   |   |-- my_wtime.F90
|   |   |-- netcdf_utils.F90
|   |   |-- p_netcdf.F90
|   |   |-- reaction.F90
|   |   |-- rnitrate.F90
|   |   |-- s_mpi.F90
|   |   |-- s_netcdf.F90
|   |   |-- serial.F90
|   |   |-- serial_fake.F90
|   |   |-- src_files_par
|   |   |-- src_files_serial
|   |   `-- sunang.F90
|   |-- moc_src
|   |   |-- constants.F90
|   |   |-- depth2press.F90
|   |   |-- f2pCO2.F90
|   |   |-- gasx.F90
|   |   |-- p2fCO2.F90
|   |   |-- p80.F90
|   |   |-- phsolvers.F90
|   |   |-- rho.F90
|   |   |-- rhoinsitu.F90
|   |   |-- singledouble.F90
|   |   |-- src_files
|   |   |-- sw_adtg.F90
|   |   |-- sw_ptmp.F90
|   |   |-- sw_temp.F90
|   |   |-- vars.F90
|   |   `-- varsolver.F90
|   |-- modules_gfortran.sh
|   |-- modules_gfortran_iris.sh
|   |-- modules_intel.sh
|   |-- modules_intel_iris.sh
|   |-- mpi_interface.h
|   |-- sdm_src
|   |   |-- MATLAB.f
|   |   |-- coupleRate.f
```

```
|   |   |-- model.f
|   |   |-- src_files
|   |   `-- vode.f
|   |-- submitFiles
|   |   |-- submit.par.cgem.sh
|   |   |-- submit.par.gd.sh
|   |   |-- submit.serial.cgem.sh
|   |   `-- submit.serial.gd.sh
|   `-- wqem_src
|       |-- Allocate_Input_WQEM.F90
|       |-- Brad_Light_Model.F90
|       |-- Flux_WQEM.F90
|       |-- INPUT_VARS_WQEM.F90
|       |-- InRemin.F90
|       |-- InitError_Check_WQEM.F90
|       |-- Init_Output_WQEM.F90
|       |-- MASS_BALANCE_WQEM.F90
|       |-- Model_Finalize_WQEM.F90
|       |-- Model_Output_WQEM.F90
|       |-- OUTPUT_NETCDF_WQEM.F90
|       |-- Read_InputFile_WQEM.F90
|       |-- Salinity_Regression_Init_WQEM.F90
|       |-- Set_Initial_Conditions_WQEM.F90
|       |-- Transport_WQEM.F90
|       |-- WQEM.F90
|       |-- WQEM_Light_Model.F90
|       |-- Write_InputFile_WQEM.F90
|       |-- carbon.F90
|       |-- diatoms.F90
|       |-- diatoms_droop.F90
|       |-- dissolved_oxygen.F90
|       |-- eut.F90
|       |-- exchange.F90
|       |-- exchange_droop.F90
|       |-- flags.F90
|       |-- greens.F90
|       |-- greens_droop.F90
```

```
|       |-- nitrog.F90
|       |-- nitrog_droop.F90
|       |-- phosph.F90
|       |-- phosph_droop.F90
|       |-- silica.F90
|       |-- src_files
|       |-- states.F90
|       `-- zoo.F90
|-- CGEM_User_Guide_V1.docx
`-- README.md
```

EPA
United States
Environmental Protection
Agency

PRESORTED STANDARD
POSTAGE & FEES PAID
EPA
PERMIT NO. G-35

Office of Research and Development (8101R)
Washington, DC 20460

Official Business
Penalty for Private Use
$300