U.S.ARMY

OVERVIEW OF CE-QUAL-W2 VERSION 5.0BETA

Zhonglong Zhang, PhD, PE, PH
Portland State University, Civil & Environmental Engineering

CE-QUAL-W2 Workshop

July 18 - 20, 2023

US Army Corps of Engineers

Environmental Systems Modeling Team

ERDC
ENGINEER RESEARCH & DEVELOPMENT CENTER

Outline

1. Overview of CE-QUAL-W2 Versions

2. CE-QUAL-W2 Capabilities
   - Hydrodynamics
   - Decoupling hydrodynamics and water quality
   - Water quality kinetics
   - Bed sediment simulation
   - Selective withdrawal

3. CE-QUAL-W2 Inputs/Outputs

CE-QUAL-W2 Versions 3.7 – 4.22

- New water quality state variables: CBOD groups, N2, TDG
- Temperature and dissolved oxygen habitat volume module
  - Determine species habitat volumes based on temperature and dissolved oxygen criteria
- Environmental performance criteria module
  - Determine volume and time weighted frequency diagrams for any state variable
- Hypolimnetic aeration module
  - Add mass rate of oxygen input to specific locations in the reservoir domain and affect local mixing if necessary
- New selective withdrawal algorithm from the USGS
- Dynamic outlet structure elevation for each structure
- Withdrawal time series outputs (seconds, minutes or hours)
- Particle tracking module
- SYSTDG module
- Sediment diagenesis, additional water quality state variables
- Post-processor W2_Post from DSI

CE-QUAL-W2 Version 4.5

- All external control files are provided in an Excel master sheet.
- Atmospheric deposition of any state variable
- Output of flow balance file, N and P mass balance file
- New generic constituent source: sediment release
- New state variables: water age, N2, dissolved total gas pressure, bacteria, CH4, H2S, SO4, Fe(II), FeOOH, Mn(II), MnO2
- New derived variables: un-ionized ammonia, TDG, turbidity, Secchi depth.
- Implementation of variable algal settling velocity
- Implementation of algal toxin production
- DOC and POC constituents with both labile and refractory groups
- Sediment diagenesis updates
- Updates to auto-port selection
- Additional outputs, etc.

CE-QUAL-W2 Version 5.0beta

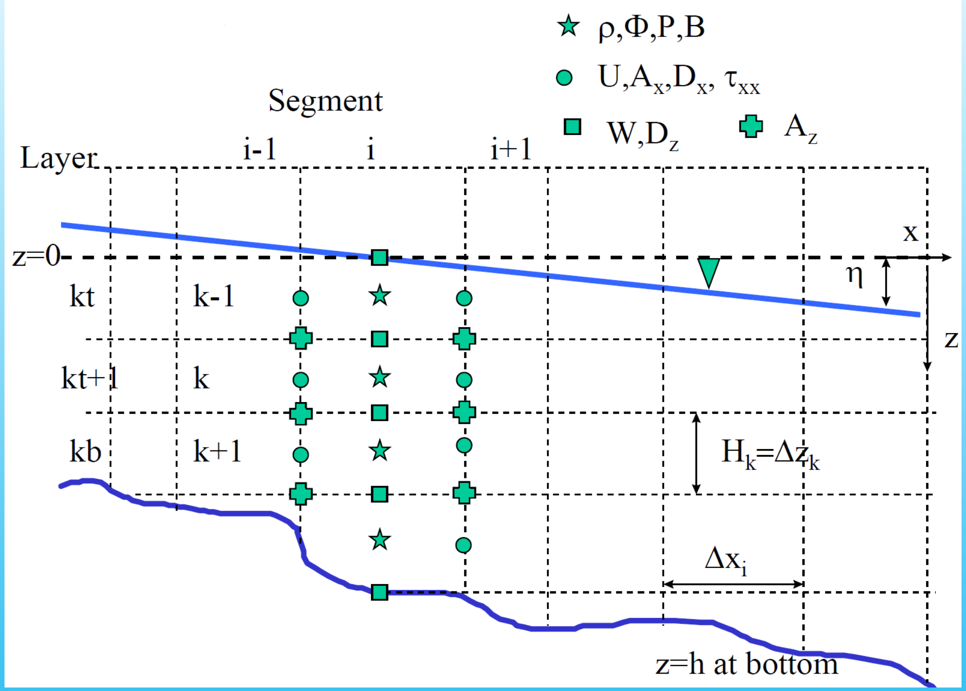
- Decouple hydrodynamics and water quality computation where direct couplings are not required
- Update selective withdrawal computation
- Write a hdf5 format output file
- Additional development and enhancement
  - ▸Anoxic carbon decomposition
  - ▸Sediment diagenesis
  - ▸New model outputs
- Hg cycle module

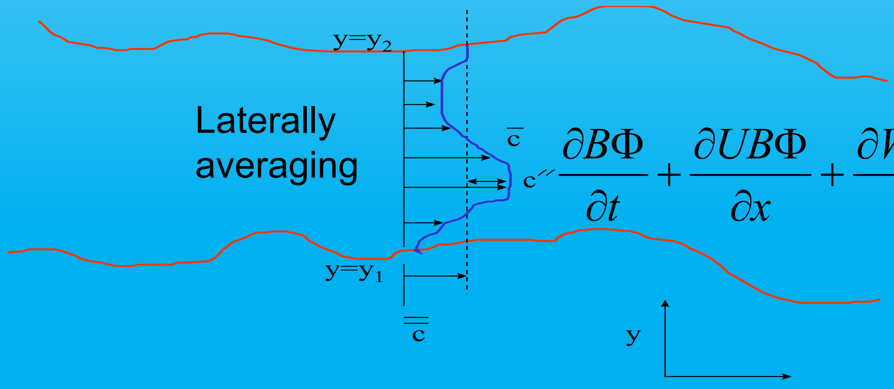
CE-QUAL-W2 Capabilities

- Ability to model multiple water bodies and branches
- Ability to model hydraulic structures and reservoir operations
- Ability to model temperature as well as many water quality constituents:
    - temperature
    - total dissolved solid
    - water age or hydraulic residence time
    - bacteria
    - nitrogen gas
    - dissolved gas pressure
    - hydrogen sulfide
    - sulfate
    - methene
    - Fe species
    - Mn species
    - inorganic phosphorus
    - ammonium
    - nitrate-nitrite
    - dissolved oxygen
    - inorganic carbon
    - alkalinity
    - silica (particulate and dissolved)
    - labile dissolved organic matter (LDOM/LDOC/LDON/LDOP)
    - refractory dissolved organic matter (RDOM/RDOC/RDON/RDOP)
    - labile particulate organic matter (LPOM/LPOC/LPON/LPOP)
    - refractory particulate organic matter (RPOM/RPOC/RPON/RPOP)
    - # of generic constituents (contaminants)
    - # of inorganic suspended solids groups
    - # of phytoplankton groups
    - # of epiphyton/periphyton groups
    - # of CBOD/CBODN/CBODP groups
    - # of zooplankton groups
    - # of macrophyte groups
    - four of algae toxins
    - Hg species (Hg0, HgII, MeHg)
    - sediment compartment

CE-QUAL-W2 Hydrodynamics and Water Quality

- State variables:
  - water level
  - vertical and horizontal velocity
  - density
  - temperature
- Water quality transport and kinetics





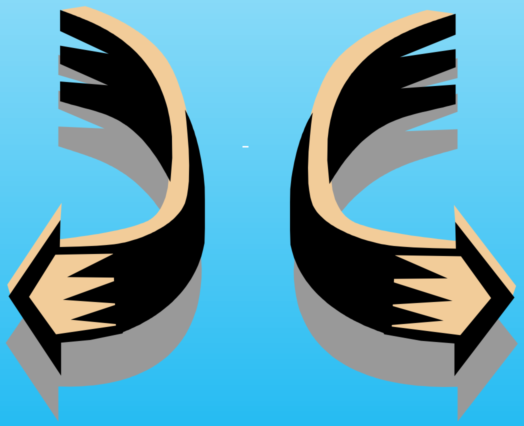
$$\frac{\partial B\Phi}{\partial t}+\frac{\partial UB\Phi}{\partial x}+\frac{\partial WB\Phi}{\partial z}-\frac{\partial\left(BD_x\frac{\partial\Phi}{\partial x}\right)}{\partial x}-\frac{\partial\left(BD_z\frac{\partial\Phi}{\partial z}\right)}{\partial z}=q_\Phi B+S_\Phi B$$

Biogeochemical Reactions and Kinetics

CE-QUAL-W2 Coupled and Decoupled Hydrodynamics and Water Quality

- Historically: two separate fields of study
- Time and space scales often differ
- Defining the time steps for simulations of hydrodynamics and water quality

Hydrodynamics

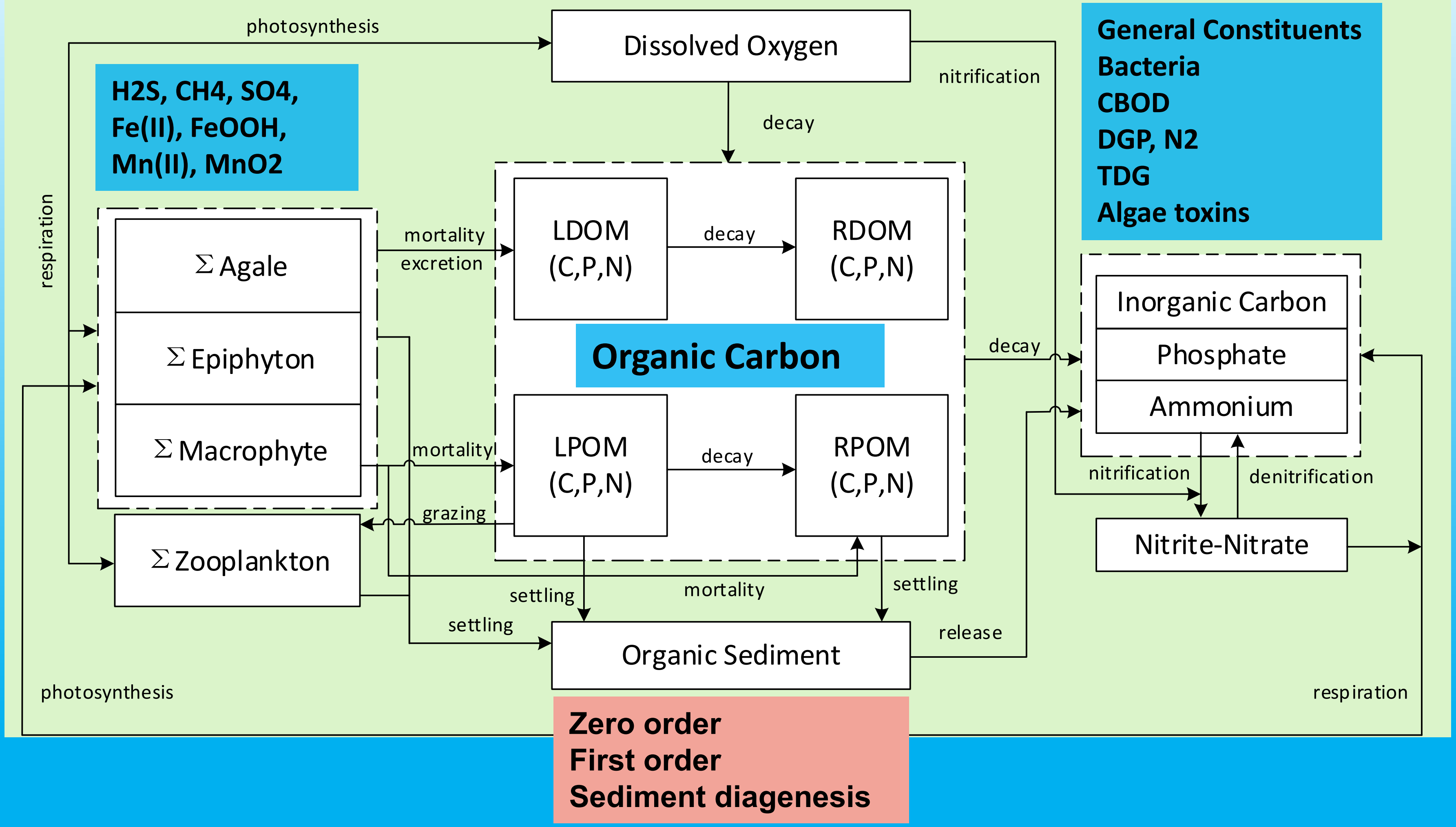


Water Quality Modeling

Maximum Time Step

$$\Delta t \leq \frac{1}{2\left(\frac{A_x}{\Delta X^2} + \frac{A_z}{\Delta Z^2}\right) + \frac{Q}{V} + \frac{\sqrt{\frac{\Delta\rho}{\rho}\frac{gH}{2}}}{\Delta X}}$$

Water Quality Kinetics



Water Quality State Variables

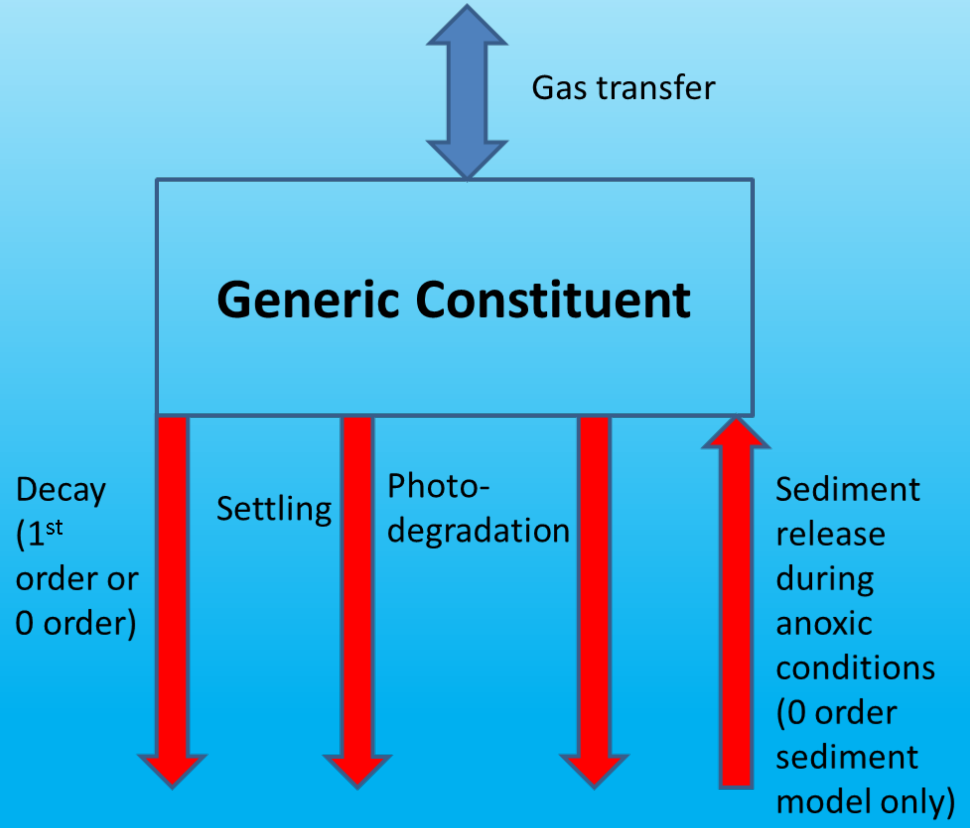
CST	CNAME2 Sh	CNAME Long name	CAC Active constituent	FMTC Fortran output format for SNP&SPR
1	TDS	"TDS, g/m^3	OFF	(f10.4)
2	Gen1-Tr	"Tracer, g/m^3	OFF	(g10.3)
3	Gen2-Cnd	"Conductivity, uS/cm	OFF	(g10.3)
4	Gen3-Cl	"Chloride, mg/l	ON	(g10.3)
5	ISS1	"ISS1, g/m^3	ON	(f10.4)
6	ISS2	"ISS2, g/m^3	ON	(f10.4)
7	WaterAge	"Age, days "	ON	(f10.4)
8	Bacteria	"Bacteria, col/100ml	OFF	(f10.4)
9	DGP	"Dissolved Gas Pressure,atm	OFF	(f10.4)
10	N2	"N2 dissolved gas, mg/l	OFF	(f10.4)
11	H2S	"H2S, dissolved gas, mg/l	ON	(f10.4)
12	CH4	"CH4 dissolved gas, mg/l	ON	(f10.4)
13	SO4	"SO4 dissolved, mg/l	ON	(f10.4)
14	FEII	"Reduced FE(II), mg/l	ON	(f10.4)
15	FEOOH	"Oxidized FeOOH, mg/l	ON	(f10.4)
16	MnII	"Reduced Mn(II), mg/l	ON	(f10.4)
17	MnO2	"Oxidized MnO2, mg/l	ON	(f10.4)
18	PO4	"Phosphate, g/m^3"	ON	(f10.4)
19	NH4	"Ammonium, g/m^3	ON	(f10.4)
20	NO3	"Nitrate-Nitrite, g/m^3	ON	(f10.4)
21	DSI	"Dissolved silica, g/m^3	OFF	(f10.4)
22	PSI	"Particulate silica, g/m^3	OFF	(f10.4)
23	LDOM	"Labile DOM, g/m^3	ON	(f10.4)
24	RDOM	"Refractory DOM, g/m^3	ON	(f10.4)
25	LPOM	"Labile POM, g/m^3	ON	(f10.4)
26	RPOM	"Refractory POM, g/m^3	ON	(f10.4)
27	ALG1	"Algae1, g/m^3	ON	(f10.4)
28	ALG2	"Algae2, g/m^3	ON	(f10.4)
29	ALG3	"Algae3, g/m^3	ON	(f10.4)
30	DO	"Dissolved oxygen, g/m^3	ON	(f10.4)
31	TIC	"Inorganic carbon, g/m^3	ON	(f10.4)
32	ALK	"Alkalinity, g/m^3	ON	(f10.4)
33	ZOO1	"Zoo1, g/m^3	ON	(f10.4)
34	LDOM-P	"LDOM P, g/m^3	ON	(f10.4)
35	RDOM-P	"RDOM P, g/m^3	ON	(f10.4)
36	LPOM-P	"LPOM P, g/m^3	ON	(f10.4)
37	RPOM-P	"RPOM P, g/m^3	ON	(f10.4)
38	LDOM-N	"LDOM N, g/m^3	ON	(f10.4)
39	RDOM-N	"RDOM N, g/m^3	ON	(f10.4)
40	LPOM-N	"LPOM N, g/m^3	ON	(f10.4)
41	RPOM-N	"RPOM N, g/m^3	ON	(f10.4)
42	MICROCYSTI	"Microcystin, g/m^3"	OFF	(g10.3)
43	CYLINDROSP	"Clindrospermopsin, g/m^3"	OFF	(g10.3)
44	ANATOXIN-A	"Anatoxin-A, g/m^3"	OFF	(g10.3)
45	SAXITOXIN	"Saxitoxin, g/m^3"	OFF	(g10.3)
46	Hg0	"Hg0, ng/L"	ON	(f10.4)
47	HgII	"HgII, ng/L"	ON	(f10.4)
48	MeHg	"MeHg, ng/L"	ON	(f10.4)

Water Quality Derived Variables

CST	CDNAME2	CDNAME	FMTCD	CDMULT
	DOC	"Dissolved organic carbon, g/m^3 "	(F10.3)	1
	POC	"Particulate organic carbon, g/m^3 "	(F10.3)	1
	TOC	"Total organic carbon, g/m^3 "	(F10.3)	1
	DON	"Dissolved organic nitrogen, g/m^3 "	(F10.3)	1
	PON	"Particulate organic nitrogen, g/m^3 "	(F10.3)	1
	TON	"Total organic nitrogen, g/m^3 "	(F10.3)	1
	TKN	"Total Kheldahl Nitrogen, g/m^3 "	(F10.3)	1
	TN	"Total nitrogen, g/m^3 "	(F10.3)	1
	NH3	"Unionized ammonia, g/m3 as N	(F10.3)	1
	DOP	"Dissolved organic phosphorus, g/m^3	(F10.3)	1
	POP	"Particulate organic phosphorus, g/m^3	(F10.3)	1
	TOP	"Total organic phosphorus, g/m^3 "	(F10.3)	1
	TP	"Total phosphorus, g/m^3 "	(F10.3)	1
	APR	"Algal production, g/m^2/day "	(F10.3)	1
	CHLA	"Chlorophyll a, mg/m^3 "	(F10.3)	1
	ATOT	"Total algae, g/m^3 "	(F10.3)	1
	%DO	"Oxygen % Gas Saturation "	(F10.3)	1
	TDG	"Total dissolved gas, % "	(F10.3)	1
	Turbidit	"Turbidity, NTU "	(F10.3)	1
	TSS	"Total suspended Solids, g/m^3 "	(F10.3)	1
	TISS	"Total Inorganic Suspended Solids,g/m^3	(F10.3)	1
	CBOD	"Carbonaceous Ultimate BOD, g/m^3	(F10.3)	1
	pH	"pH "	(F10.3)	1
	CO2	"CO2 "	(F10.3)	1
	HCO3	"HCO3 "	(F10.3)	1
	CO3	"CO3 "	(F10.3)	1
	Secchi	"Secchi disk depth, m "	(F10.3)	1
	PHgIIw	"Particulate HgII-w, ng/l"	(F10.4)	1
	PHgIIs	"Particulate HgII-s, ng/g"	(F10.4)	1
	PMeHgw	"Particulate MeHg-w, ng/l"	(F10.4)	1
	PMeHgs	"Particulate MeHg-s, ng/g"	(F10.4)	1
	DHgII	"Dissolved HgII, ng/l"	(F10.4)	1
	DMeHg	"Dissolved Me Hg, ng/l"	(F10.4)	1

Generic Constituents

$$S_g = -K_0\theta^{(T-20)} - K_1\theta^{(T-20)}\Phi_g - \omega_g\frac{\partial\Phi_g}{\partial z} - \alpha I_o(1-\beta)e^{-\lambda z}\Phi_g + \frac{A_{sur}}{V_{sur}}K_L\left(\Phi_s - \Phi_g\right) + \boxed{K_{sedrel}SOD\frac{A}{V}}$$

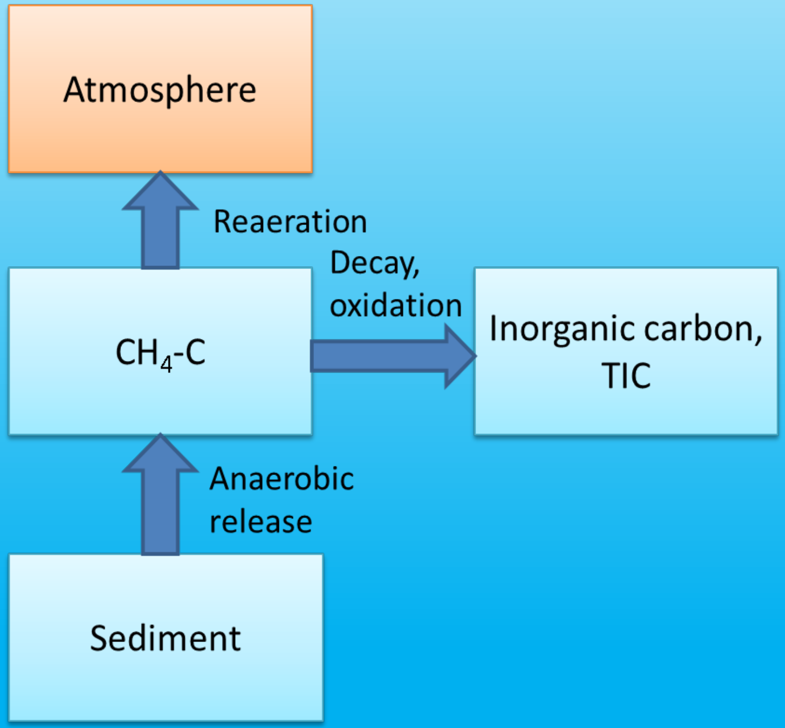


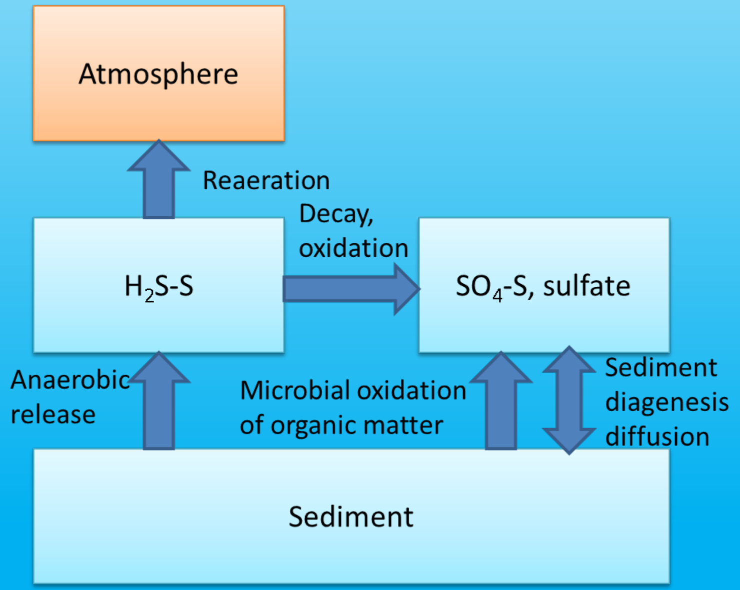
GENERIC CONSTITUENT	CG1
CGQ10, Arrhenius temperature rate multiplier, theta	0
CG0DK, 0-order decay rate, with mass concentration units: gm-3day-1	0
CG1DK 1st -order decay rate, day-1	0
CGS Settling rate, m day-1	0
CGLDK Photodegradation parameter, m2J-1	0
CGKLF Fraction of surface reaeration coefficient, KL, for dis-solved oxyger	0
CGS Gas transfer saturation concentration, mg/l	0
CGR, sediment release rate as a fraction of zero order SOD	0

CH_4, H_2S, SO_4

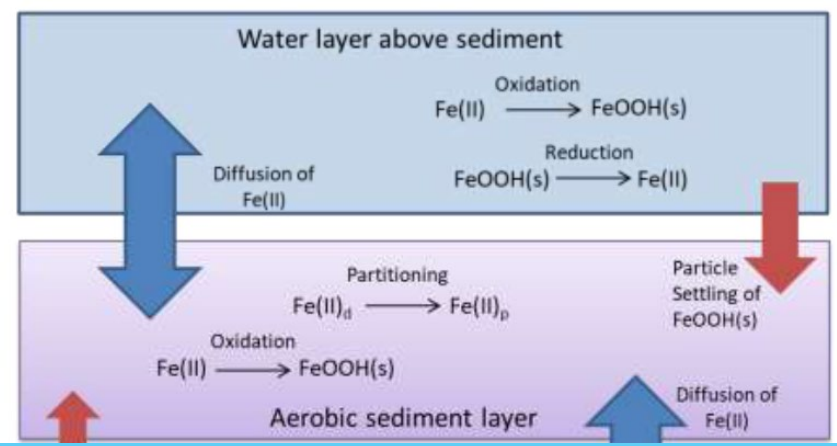
$$S = \boxed{\underbrace{SOD\,\gamma_{OM}\,\delta_{SODR}\,\frac{A_{sed}}{V}}_{\text{0-order sediment release}}} + \underbrace{A_{sur}\,K_L\,(-\Phi)}_{\text{reaeration}} - \underbrace{\Theta^{T-20}\,K\,\Phi_C}_{\text{decay}}$$

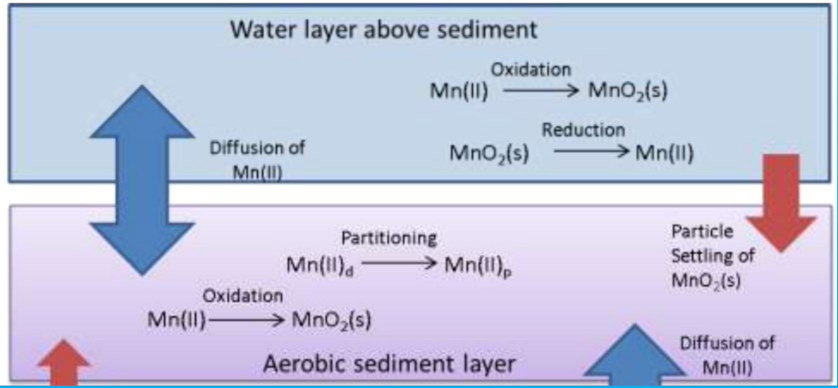
H2S	WB1
H2SR, sediment release rate, fraction of SOD (zero order),[-]	0.01
H2SQ10, Arrhenius temperature rate multiplier, theta	1.04
H2S1DK, first order decay rate, day-1	0.001
SO4R, sediment release of SO4, source, fraction of SOD (zero order), [-]	0.001
CH4	WB1
CH4R, methane sediment release rate, fraction of SOD (zero order), [-]	0.01
CH4Q10, Arrhenius temperature rate multiplier, theta	1.04
CH41DK, first order decay rate, day-1	0.1





Fe(II), FeOOH, Mn(II), MnO_2



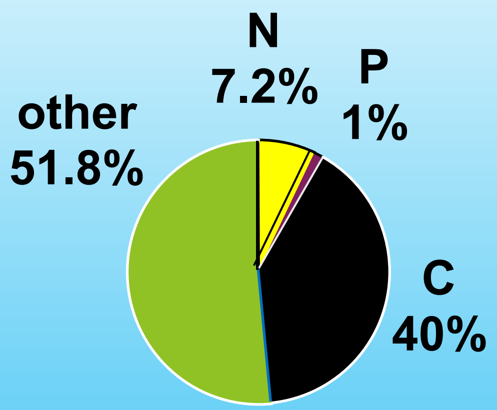


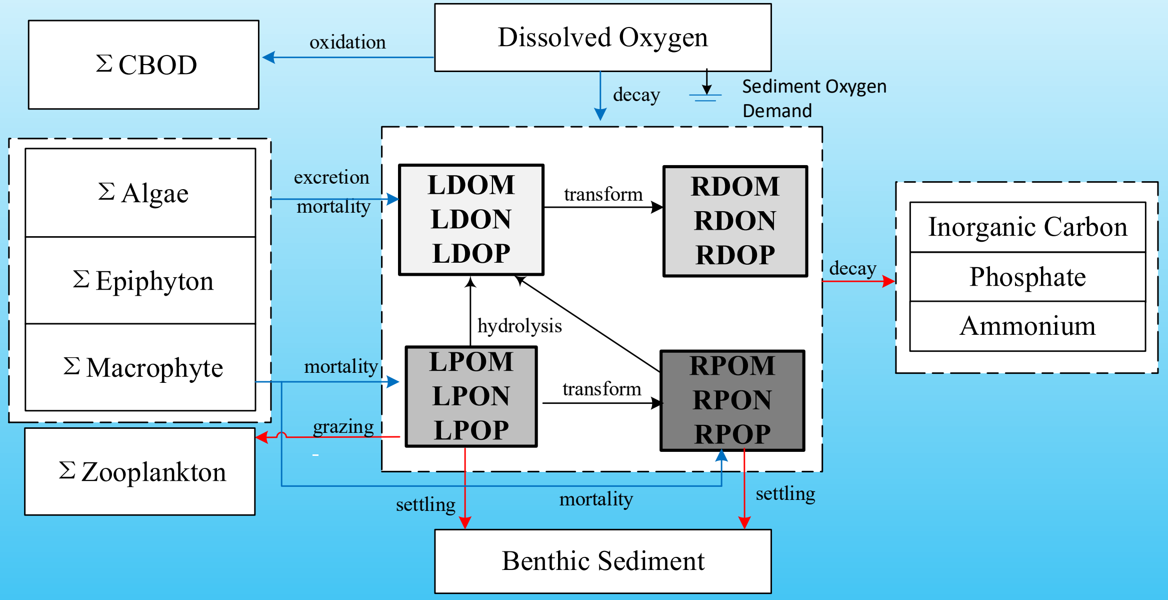
$$S_{MnII} = -K_{Mn}\Phi_{DO}\theta^{(PH-7)}\Phi_{MnII} + K_{MnO2}\frac{K_{MnO2}}{K_{MnO2}+\Phi_{DO}}\Phi_{MnO2} + K_{sedrel}SOD\frac{A}{V}$$

$$S_{FeII} = -K_{Fe}\Phi_{DO}\theta^{(PH-7)}\Phi_{FeII} + K_{FeOOH}\frac{K_{FeOOH}}{K_{FeOOH}+\Phi_{DO}}\Phi_{FeOOII} + K_{sedrel}SOD\frac{A}{V}$$

Fe(II) and FeOOH	WB1
FEIIR Sediment release rate of reduced Fe, a fraction of SOD for the zero order SOD model only [-]	0.001
KFE_OXID Rate of Fe oxidation under oxic conditions, m3 d-1 g-1	1
KFE_RED Rate of iron reduction under anaerobic conditions, day-1	4
KFEOOH_HalfSat Half-saturation constant for O2 for FeOOH reduction to Fe(II) g/m3	0.2
FeSetVel Settling velocity of Fe oxide, m/day	0.001
Mn(II) MnO2	WB1
MNIIR Sediment release rate of reduced Mn, a fraction of SOD for the zero order SOD model only [-]	0.001
KMN_OXID Rate of Mn oxidation under oxic conditions, day-1	0.01
KMN_RED Rate of Mn reduction under anaerobic conditions, day-1	0.001
KFMNOH_HalfSat Half saturation constant for Mn oxidation	0.01
MNSetVel Settling velocity of Mn oxide, m/day	0.1

Organic Matter (OM/OC) Constituents

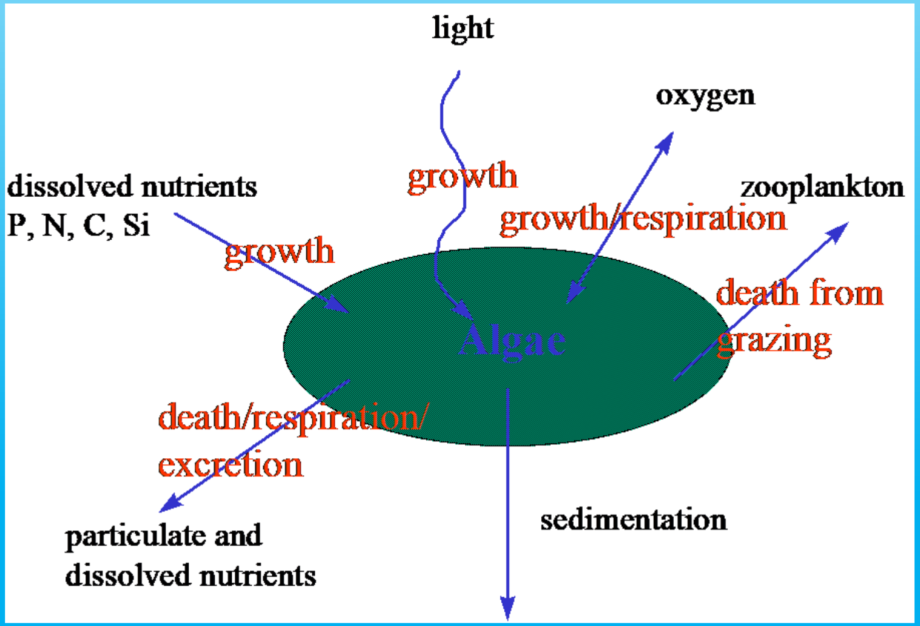




- Labile Particulate Organic Constituents (LPOC/LPON/LPOP)
- Refractory Particulate Organic Constituents (RPOC/RPON/RPOP)
- Labile Dissolved Organic Constituents (LDOC/LDON/LDOP)
- Refractory Dissolved Organic Constituents (RDOC/RDON/RDOP)

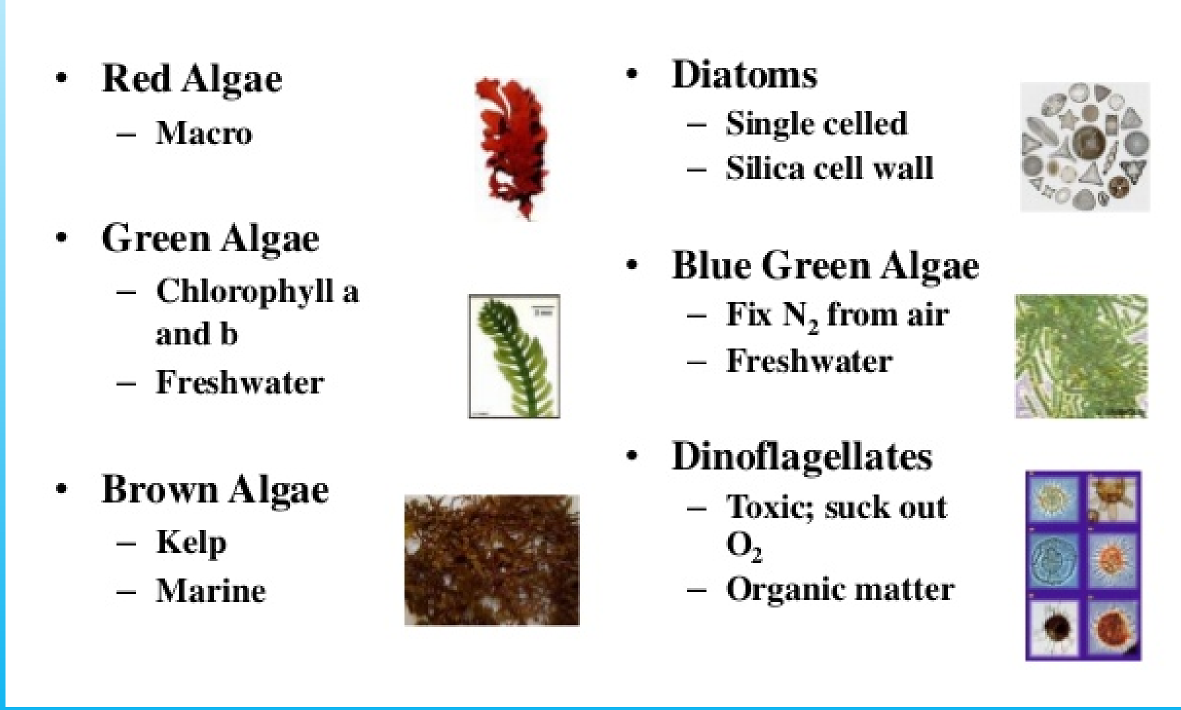
Algae Groups and Toxins

- Multi- Phytoplankton
- Multi- Epiphyton
- Multi- Macrophytes
- Four Algae Toxins



ALGAL RATES	ALG1
AG - algae max growth rate- 1/day	2
AR - algae respiration rate- 1/day	0.04
AE - algae excretion rate	0.04
AM - algae mortality rate	0.1
AS - algae settling velocity- m/day	0.1
AHSP - algae half-saturation rate for P- mg/l	0.003
AHSN - algae half-saturation rate for N- mg/l	0.014
AHSSI - algae half-saturation for Si- mg/l	0
ASAT - algae light saturation- W/m2	100
AT1 - Temperature C for set point 1	5
AT2 - Temperature C for set point 2	30
AT3 - Temperature C for set point 3	35
AT4 - Temperature C for set point 4	40
AK1 - fraction of max growth rate at AT1	0.1
AK2 - fraction of max growth rate at AT2	0.99
AK3 - fraction of max growth rate at AT3	0.99
AK4 - fraction of max growth rate at AT4	0.1
AP ALGP Stoichiometric ratio of P to algae biomass	0.005
AN ALGN Stoichiometric ratio of N to algae biomass	0.08
AC ALGC Stoichiometric ratio of C to algae biomass	0.45
ASI ALGSI Stoichiometric ratio of Si to algae biomass	0
ACHLA Chlorophyll a to algae biomass ratio	0.065
APOM ALPOM fraction of biomass going to POM at death	0.8
ANEQN NH4-NO3 preference equation #	1
ANPR Parameter for ANEQN#2	0.001
O2AR Stoichiometric ratio of O2 to algae biomass, for algal respiration (mg O2/	1.1
O2AG Stoichiometric ratio of O2 to algae biomass, for algal primary production	1.4
Algae Vertical Migration, ON/OFF, AVERTM	OFF

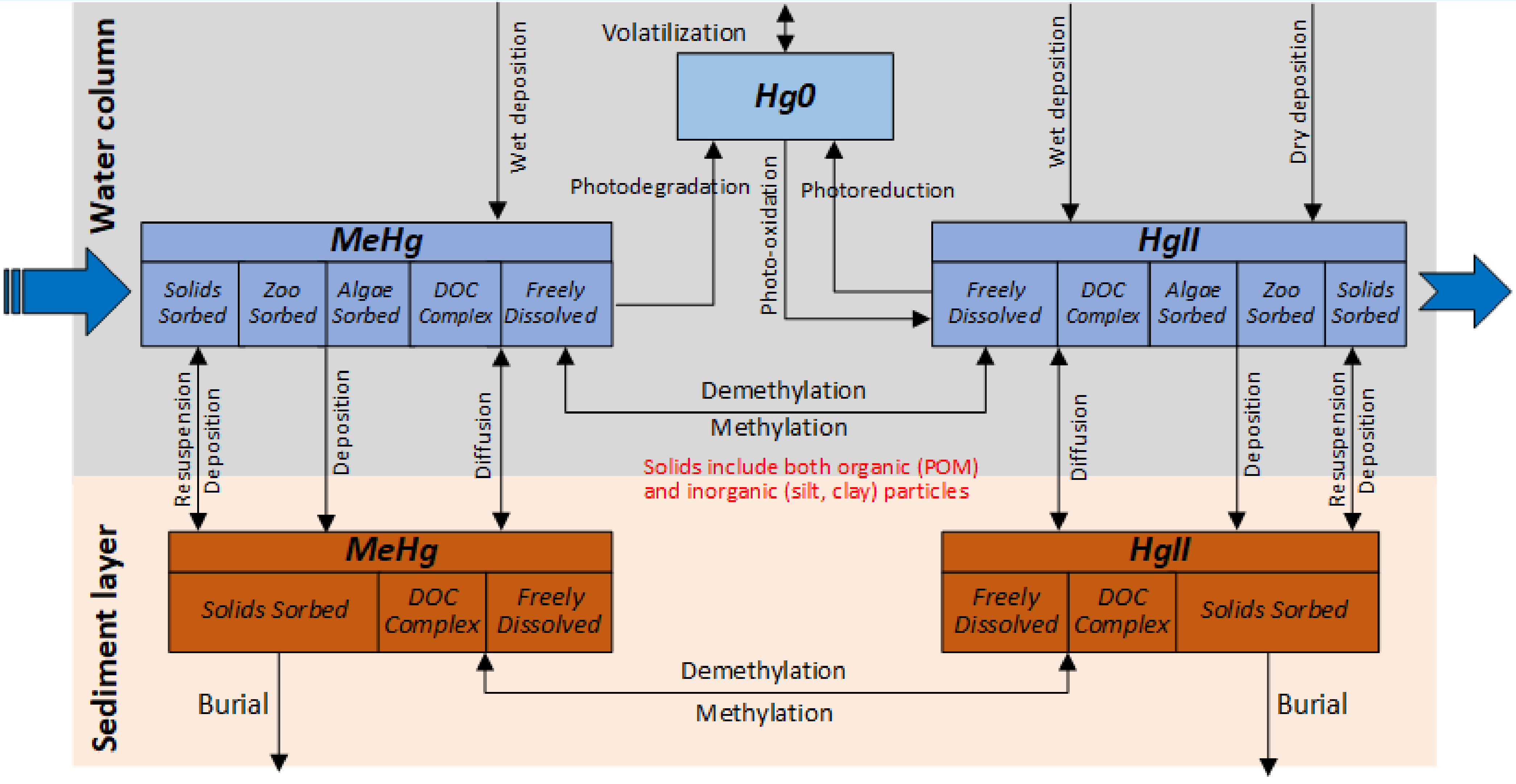
Algae Groups and Toxins



1	AlgaeMigration: ON/OFF									
2	ON									
3	NumAlgae	Debug Output(1-ON/0-OFF)								
4	1	1								
5	AlgaeGroup - repeat for each NumAlgaeGroups									
6	1									
7	NumMigrateIntervals - # of intervals for algal migration (Models 1 and 2 only)									
8	1									
9	JDAYStart - start of each migration interval									
10	1									
11	JDAYend									
12	800									
13	ContiuumModel: 1 - velocity time; 2 - velocity time and space; 3 - density growth; 4 - density growth (Visser)									
14	1									
15	Amplitude(	PhaseShift(	Calibration	DepthCalc(	ExpDepth((	DepthLimit	DepthLimit	LossFractic	Parameters of Model	
16	2	1.570796	0.4	0	12.5	0	25	0.05		
17	ColonyRad	MinColony	MaxColony	InitColonyI	InitColonyI	DecayTime	DecayTime	CoeffDenIr	CoeffDenD	DepthLimit
18										
19	ColonyRad	MinColony	MaxColony	InitColonyI	InitColonyI	CompIrrad	CoeffDenIr	CoeffDenIr	CoeffDenD	CoeffDenD
20										

1	Cyanotoxins Control File	ON/OFF	DEBUG
2	TOXINCONTROL: ATOX (turn ON/OFF all algae toxins),ATOX_DEBUG (turn on d	ON	ON
3	MICROCYSTIN	ALG1	ALG2
4	CTP_MC, fraction of algae concentration producing MC	0.5	0.25
5	CTB_MC, ratio of intracellular toxin to dry weight biomass (mg toxin/mg DW)	0.1	0.2
6	CTR_MC, release rate, day-1	0.5	
7	CTD_MC, extracellular decay , day-1	0.1	
8	CYLINDROSPERMOPSIN	ALG1	ALG2
9	CTP_CYN, fraction of algae concentration producing CYN	1	0
10	CTB_CYN, ratio of intracellular toxin to dry weight biomass (mg toxin/mg DW)	0.25	0.2
11	CTR_CYN, release rate, day-1	0.5	
12	CTD_CYN, extracellular decay , day-1	0.25	
13	ANATOXIN-A	ALG1	ALG2
14	CTP_ATX, fraction of algae concentration producing ATX	0.5	0.25
15	CTB_ATX, ratio of intracellular toxin to dry weight biomass (mg toxin/mg DW)	0.1	0.2
16	CTR_ATX, release rate, day-1	0.5	
17	CTD_ATX, extracellular decay, day-1	0.1	
18	SAXITOXIN	ALG1	ALG2
19	CTP_STX, fraction of algae concentration producing STX	0.5	0.25
20	CTB_STX, ratio of intracellular toxin to dry weight biomass (mg toxin/mg DW)	0.1	0.2
21	CTR_STX, release rate, day-1	0.5	
22	CTD_STX, extracellular decay , day-1	0.1	

Hg Cycling and Kinetics



Hg Species and Forms

Hg form	Phases	
	Dissolved	Particulate
Inorganic mercury Hg(II)	X	X
Methylmercury MeHg	X	X
Elementary mercury Hg(0)	X	

Hg Kinetic Sources and Sinks

- Hg0 photo-oxidation
- HgII photo-reduction
- MeHg photo-degradation
- Hg0 volatilization

- Hg0 photo-oxidation
- Biological demethylation
- Photo-reduction
- Methylation
- Settling of sorbed fractions
- Diffusion across the sediment-water interface

- Methylation
- Photodegradation
- Volatilization
- Biological Demethylation
- Settling of sorbed fractions
- Diffusion across the sediment-water interface

Water Quality: Derived Variables

Turbidity (NTU) is computed from a correlation to TSS (Total Suspended Solids)

$$Turbidity = e^{A+ln(TSS)} + B$$

Secchi disk (m) is computed from λ (light extinction coefficient)

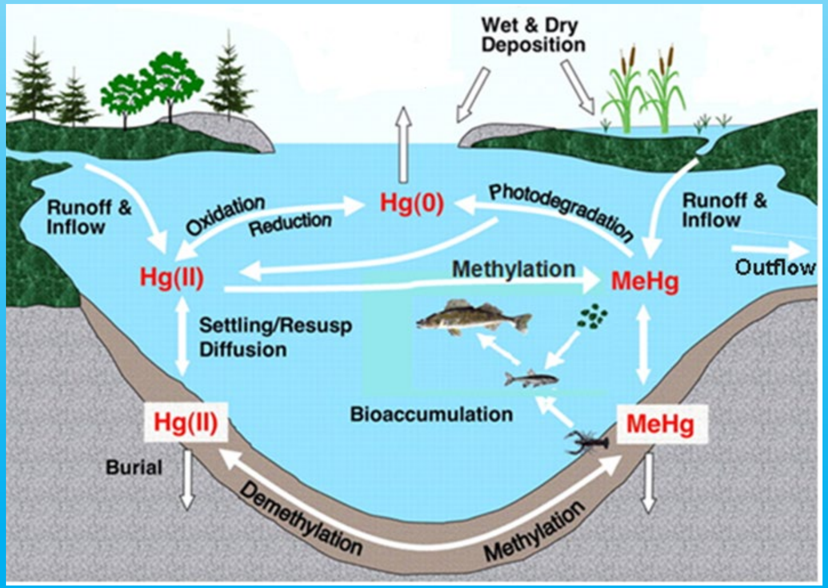
$$Secchi = \frac{A}{\lambda}$$

Dissolved and particulate Hg species

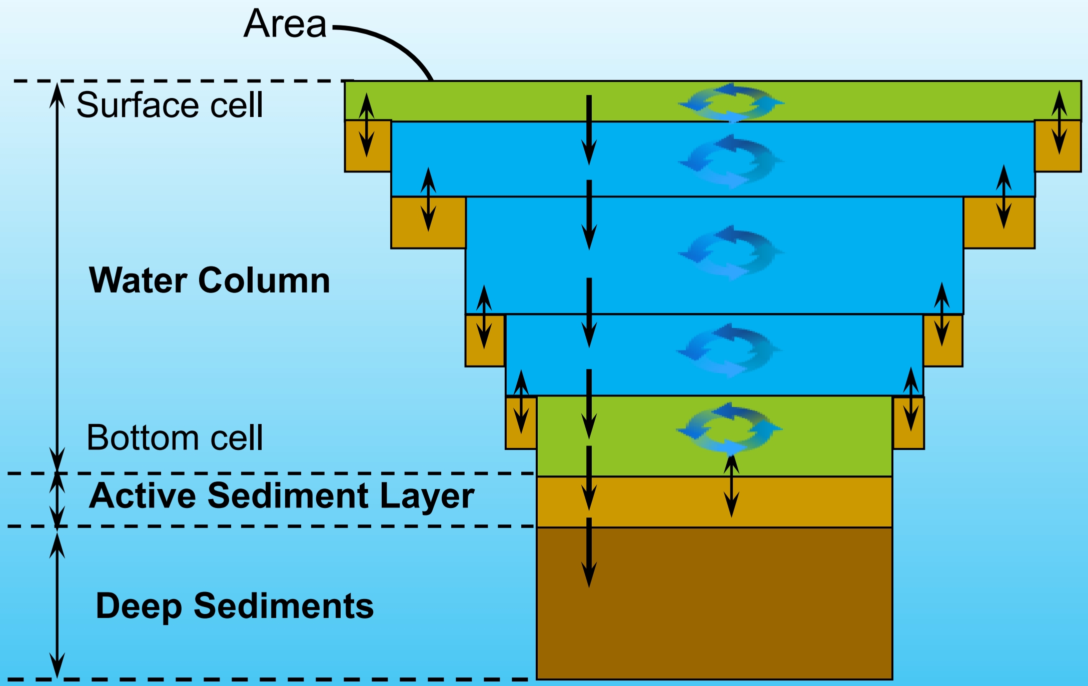
Sediment Compartment

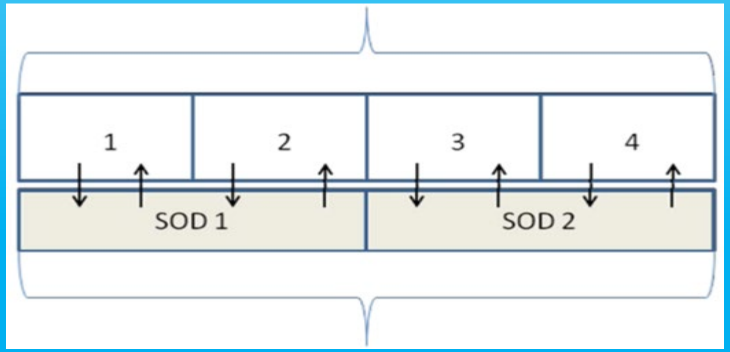
Active sediment layer in Hg module

- Directly specify Hg releases from the sediment, with temperature adjustment
- Internally calculate mass transfer of chemicals



Courtesy of USEPA





Sediment Compartment

Zero order sediment fluxes

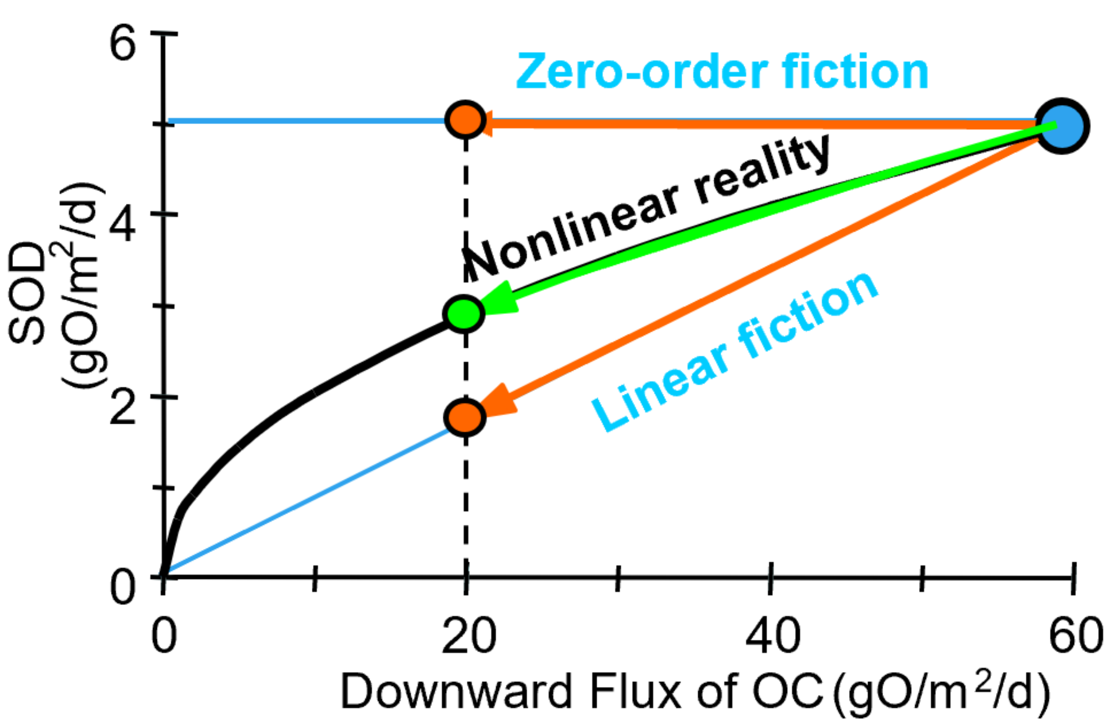
- Directly specify nutrient releases, with temperature adjustment
- Available in almost all water quality models

First order sediment fluxes

- Link fluxes to organic matter
- Limited application

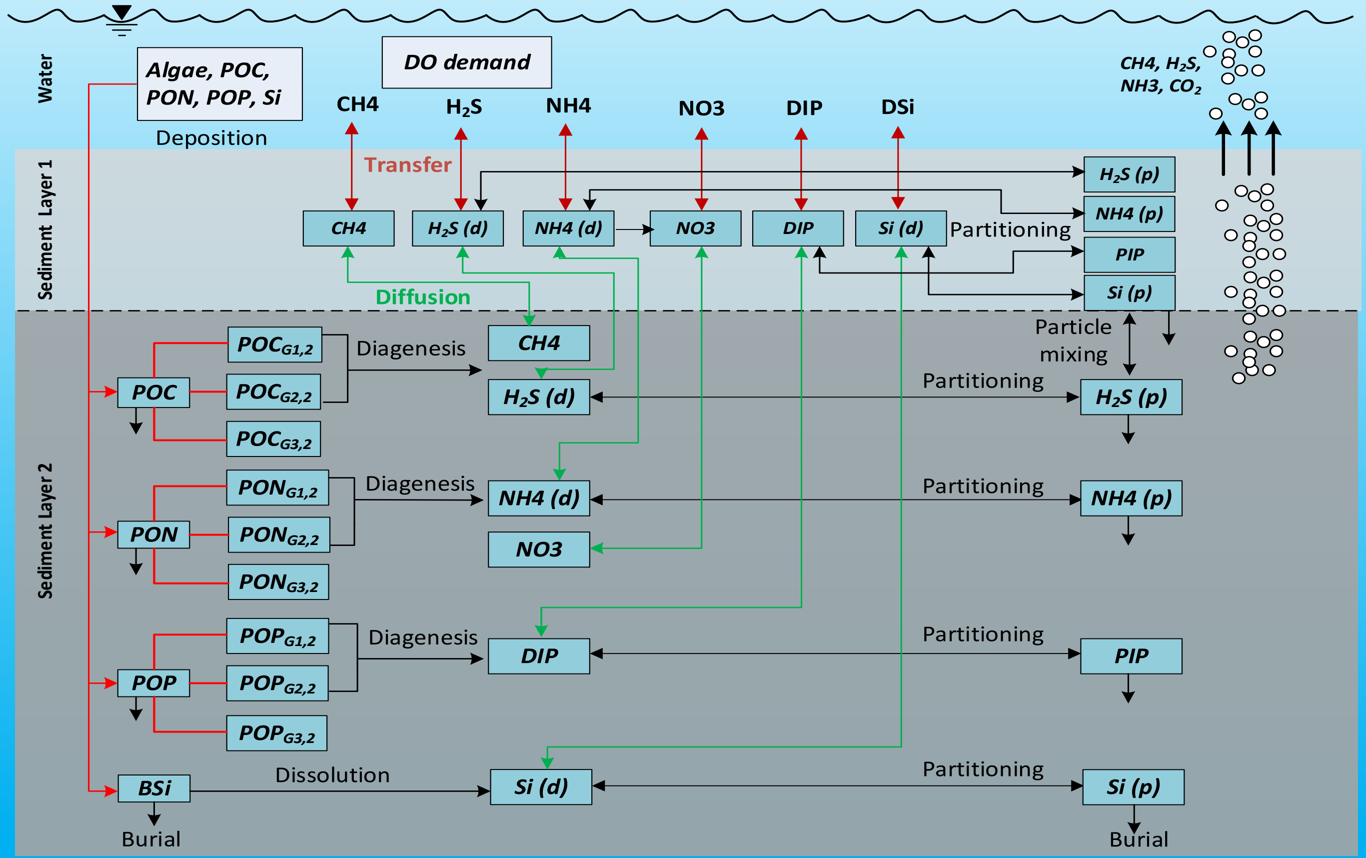
Sediment diagenesis modeling

- Directly simulate the reactions in the sediment layer



Courtesy of Steven Chapra

Sediment Diagenesis



- Organic matter (OM) accumulates on the bottom of water bodies
- Accumulated OM reactions in bottom sediment layer
  - Aerobic reactions - fast
  - Anaerobic reactions – slow
- Sediment fluxes
  - Any dissolved materials may move between water and sediment pore water
  - DO from water to sediment → SOD
  - Mass flux depends on concentration gradient

Sediment Diagenesis Parameters and Calibration

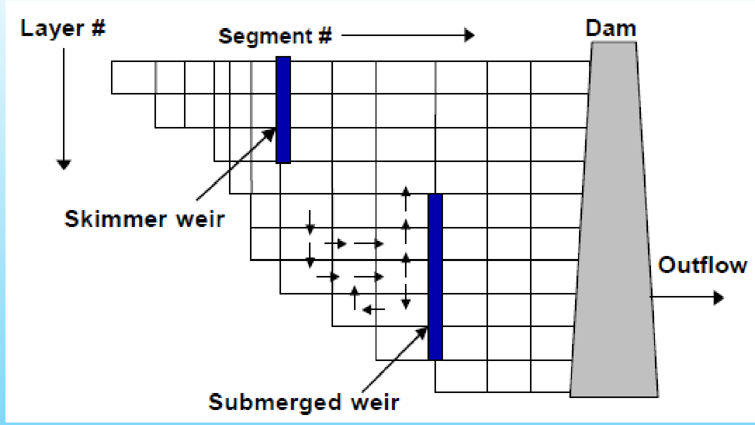
$ W2_diagenesis input file			
$ All lines at top of file starting with $ are comments and disregarded by the model			
$ Additional inputs are required if a group switch is ON			
$ Zhong Zhang, 7/21/21			
"Global Switch for all sediment diagenesis features"	.TRUE.		
"Include FFT layer (Fine Fluids Tailing - for Pit Lakes)"	.FALSE.		
"FFT layer number of periods"	5		
"FFT layer start times"	1	65	12
"FFT layer end times"	50	100	17
"Initial tailings concentration in FFT (gm/m3)"	360000		
"Sediment settling velocity of FFT to MFT (m/d)"	0		
"Move FFT layer during consolidation"	.FALSE.		
"Include bed consolidation"	.FALSE.		
"Fraction of layer thickness at which water layer is added	1		
"Number of bed consolidation regions"	6		
"Starting segment for regions"	1	14	3
"Ending segment for regions"	13	35	5
"Data type for bed consolidation for each region (0: Const	1	1	
"Bed consolidation rate (m/d)"	0	0	
"Bed consolidation data file"	Regn.npt		
"Write bed elevation snapshot output"	.FALSE.		
"Write bed porosity snapshot output"	.FALSE.		
"Include sediment diagenesis simulation"	.TRUE.		
"Initial bed thickness in meters"	0.2		
"Initial sediment bed porosity"	0.8		
"Sediment bed particle size in microns"	100		
"Sediment type (1: Cohesive, 2: Non-cohesive)"	2		
"Sediment bulk density (kg/m3)"	2650		
"Sediment particle settling velocity (m/d)"	5		
"Include sediment resuspension and deposition process	.FALSE.		
"Include bubble release"	.FALSE.		
"Gas diffusion coefficient in sediment in m/s"	1.0d-9		
"Calibration parameter R1 in m"	0.0014		
"Young's modulus E in N/m2"	1.4d+9		
"Critical stress intensity factor for sediments K1c in N/m^3	300		
"Bubbles release scale"	0		
"Fraction of critical pressure at which cracks close"	0.2		
"Switch to limit bubble size"	.TRUE.		
"Maximum bubble radius in mm"	80		
"Switch to use slow release of bubbles"	.TRUE.		
"Bubbles release fraction (sediments)"	0.001		
"Bubbles accumulation fraction"	0.1		
"Number of bubbles release array"	2000		
"Bubbles release fraction (atmosphere)"	0.001		
"Bubbles-water gas exchange rate (1/s)"	1.0d-7		
"Apply additional turbulence due to bubbles release"	.FALSE.		
"Turbulence scaling factor for bubbles release"	0.001		
"Include POM resuspension"	.FALSE.		
"Critical shear stress for POM resuspension dynes/cm^2"	0.001		
"Critical Shields parameter for POM"	10		
"Use Cao method to estimate critical Shields parameter (rather than using input value)"	.FALSE.		
"POM specific gravity"	1.5		
"POM particle diameter m"	0.0001		
"Include modeling of alkalinity/pH in sediments"	.FALSE.		
"Include modeling of Iron (FeOOH and Fe(II)) in sediment	.FALSE.		
"Include modeling of Manganese (Mn(II) and MnO2) in se	.FALSE.		
"Number of regions for different initial sediment concent	6		

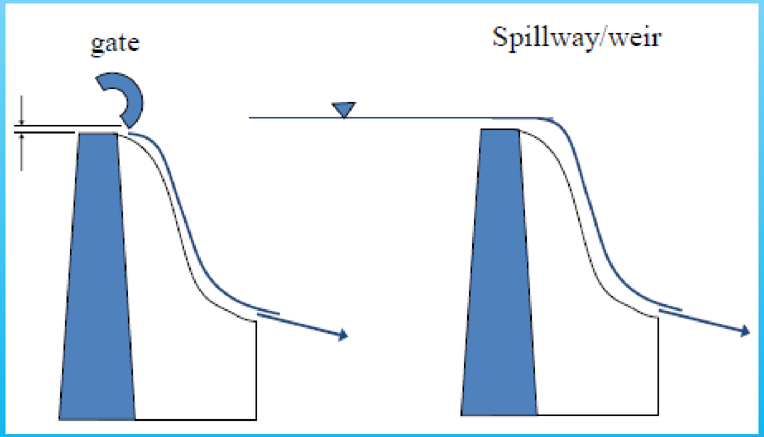
	Region1	Region2	Region3	Region4	Region5		
"Starting segment for regions"	1	14	36	54	67	82	1
"Ending segment for regions"	13	35	51	66	81	90	2
"Fraction of labile POC"	0.1	0.1	0.1	0.1	0.1	0.1	3
"Fraction of refractory POC"	0.89	0.89	0.89	0.89	0.89	0.89	4
"Fraction of labile PON"	0.1	0.1	0.1	0.1	0.1	0.1	5
"Fraction of refractory PON"	0.89	0.89	0.89	0.89	0.89	0.89	6
"Fraction of labile POP"	0.1	0.1	0.1	0.1	0.1	0.1	7
"Fraction of refractory POP"	0.89	0.89	0.89	0.89	0.89	0.89	8
"Pore water diffusion coefficient m2/d"	0.0025	0.0025	0.0025	0.0025	0.0025	0.0025	9
"Particle mixing velocity between aerobic and anaerobic l	0.00006	0.00006	0.00006	0.00006	0.00006	0.00006	10
"Burial velocity m/d"	0.000274	0.000274	0.000274	0.000274	0.000274	0.000274	11
"Reference POC G1 concentration for bioturbation mg-C/g	0.01	0.01	0.01	0.01	0.01	0.01	12
"CH4 production calculation method (0: Analytical 1: Num	1	1	1	1	1	1	13
"DO threshold for aerobic layer oxidation rates mgO2/L"	2	2	2	2	2	2	14
"Nitrification rate in aerobic layer at DO below threshold	0.3	0.3	0.3	0.3	0.3	0.3	15
"Nitrification rate in aerobic layer at DO above threshold	0.3	0.3	0.3	0.3	0.3	0.3	16
"Denitrification rate in aerobic layer at DO below thresho	0.1	0.1	0.1	0.1	0.1	0.1	17
"Denitrification rate in aerobic layer at DO above thresho	0.1	0.1	0.1	0.1	0.1	0.1	18
"Denitrification rate in anerobic layer m/d"	0.1	0.1	0.1	0.1	0.1	0.1	19
"CH4 oxidation rate in aerobic layer m/d"	0.7	0.7	0.7	0.7	0.7	0.7	20
"Half-saturation oxygen constant for CH4 oxidation mg-O2	0	0	0	0	0	0	21
"Nitrification half-saturation constant for NH4 in aerobic	0.728	0.728	0.728	0.728	0.728	0.728	22
"Nitrification half-saturation constant for O2 in aerobic la	0.37	0.37	0.37	0.37	0.37	0.37	23
"Temperature coefficient for pore water diffusion betwee	1.08	1.08	1.08	1.08	1.08	1.08	24
"Temperature coefficient for particle mixing diffusion coe	1	1	1	1	1	1	25
"Temperature coefficient for nitrification"	1.123	1.123	1.123	1.123	1.123	1.123	26
"Temperature coefficient for denitrification"	1.08	1.08	1.08	1.08	1.08	1.08	27
"Temperature coefficient for methane oxidation"	1.079	1.079	1.079	1.079	1.079	1.079	28
"SO4 concentration above which sulfide over methane is	20	20	20	20	20	20	29
"H2S oxidation rate in aerobic layer m/d"	0.2	0.2	0.2	0.2	0.2	0.2	30
"Temperature coefficient for H2S oxidation"	1.079	1.079	1.079	1.079	1.079	1.079	31
"H2S oxidation normalization constant for O2 mgO2/L"	4	4	4	4	4	4	32
"Diagenesis rate for labile POC (G1) 1/d"	0.035	0.035	0.035	0.035	0.035	0.035	33
"Diagenesis rate for refractory POC (G2) 1/d"	0.0018	0.0018	0.0018	0.0018	0.0018	0.0018	34
"Diagenesis rate for inert/slow refractory POC (G3) 1/d"	0	0	0	0	0	0	35
"Diagenesis rate for labile PON (G1) 1/d"	0.035	0.035	0.035	0.035	0.035	0.035	36
"Diagenesis rate for refractory PON (G2) 1/d"	0.0018	0.0018	0.0018	0.0018	0.0018	0.0018	37
"Diagenesis rate for inert/slow refractory PON (G3) 1/d"	0	0	0	0	0	0	38
"Diagenesis rate for labile POP (G1) 1/d"	0.035	0.035	0.035	0.035	0.035	0.035	39
"Diagenesis rate for refractory POP (G2) 1/d"	0.0018	0.0018	0.0018	0.0018	0.0018	0.0018	40
"Diagenesis rate for inert/slow refractory POP (G3) 1/d"	0	0	0	0	0	0	41
"Temperature coefficient for labile POC"	1.1	1.1	1.1	1.1	1.1	1.1	42
"Temperature coefficient for refractory POC"	1.15	1.15	1.15	1.15	1.15	1.15	43
"Temperature coefficient for inert/slow refractory POC"	1	1	1	1	1	1	44
"Temperature coefficient for labile PON"	1.1	1.1	1.1	1.1	1.1	1.1	45
"Temperature coefficient for refractory PON"	1.15	1.15	1.15	1.15	1.15	1.15	46
"Temperature coefficient for inert/slow refractory PON"	1	1	1	1	1	1	47
"Temperature coefficient for labile POP"	1.1	1.1	1.1	1.1	1.1	1.1	48
"Temperature coefficient for refractory POP"	1.15	1.15	1.15	1.15	1.15	1.15	49
"Temperature coefficient for inert/slow refractory POP"	1	1	1	1	1	1	50
"PO4 sorption coefficient in anaerobic layer m^3/kg"	0.02	0.02	0.02	0.02	0.02	0.02	51
"Incremental PO4 partition coefficient"	0	0	0	0	0	0	52
"Critical oxygen concentration for incremental sorption mg	0.01	0.01	0.01	0.01	0.01	0.01	53
"NH4 sorption coefficient in aerobic layer m^3/kg"	0.001	0.001	0.001	0.001	0.001	0.001	54
"NH4 sorption coefficient in anaerobic layer m^3/kg"	0.001	0.001	0.001	0.001	0.001	0.001	55
"H2S sorption coefficient in aerobic layer m^3/kg"	0.1	0.1	0.1	0.1	0.1	0.1	56
"H2S sorption coefficient in anaerobic layer m^3/kg"	0.1	0.1	0.1	0.1	0.1	0.1	57
"Algorithm for POM resuspension (0: Wind induced resuspension, 1: Bottom scour resuspension) Only used if Include POM resuspension is .TRUE."	1	0					58
"Fe(II) sorption coefficient in aerobic layer m^3/g"	0.00005	0.00005					59
"Fe(II) sorption coefficient in anaerobic layer m^3/g"	0.01	0.01					60
"Mn(II) sorption coefficient in aerobic layer m^3/g"	0.00005	0.00005					61
"Mn(II) sorption coefficient in anaerobic layer m^3/g"	0.01	0.01					62
"Write sediment fluxes"	.TRUE.						
"Frequency of output days"	1						

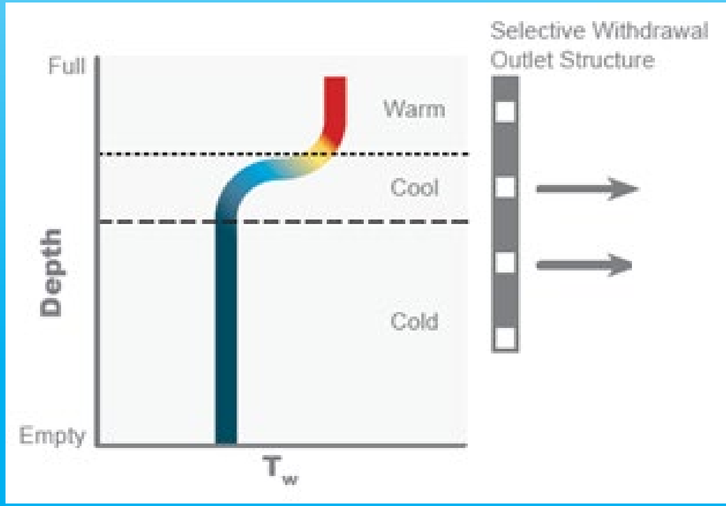
- Complex, uncertainty in sediment diagenesis parameter values which are often expensive to obtain and are heterogeneous, can lead to longer simulation times
- Seems like a lot of parameters
- What do we calibrate?
  - Net settling rates
  - Burial rates
  - Particle splits (G1, G2, G3)
  - Phosphate partition coefficients.
- References
  - *Di Toro, D.M. 2000. Sediment Diagenesis Modeling. New York, John-Wiley.*
  - *http://www.gonzo.cbl.umces.edu/index.htm*

Hydraulic Structures and Withdrawal

- Spillways
- Gates (including sluice gates)
- Pipes (including internal hydraulics for 1D unsteady flow)
- Internal/ Floating weirs
- Pumps or flow-based water level control
- Selective withdrawals for blending of warmer and colder waters to meet targeted water quality

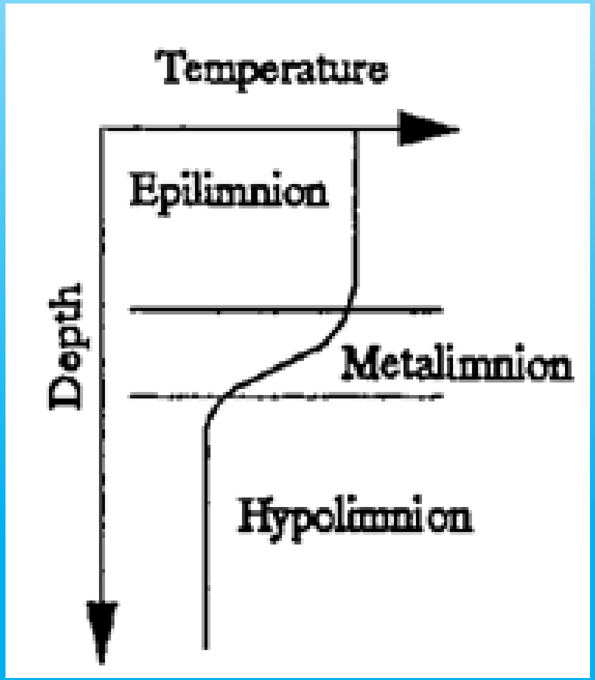


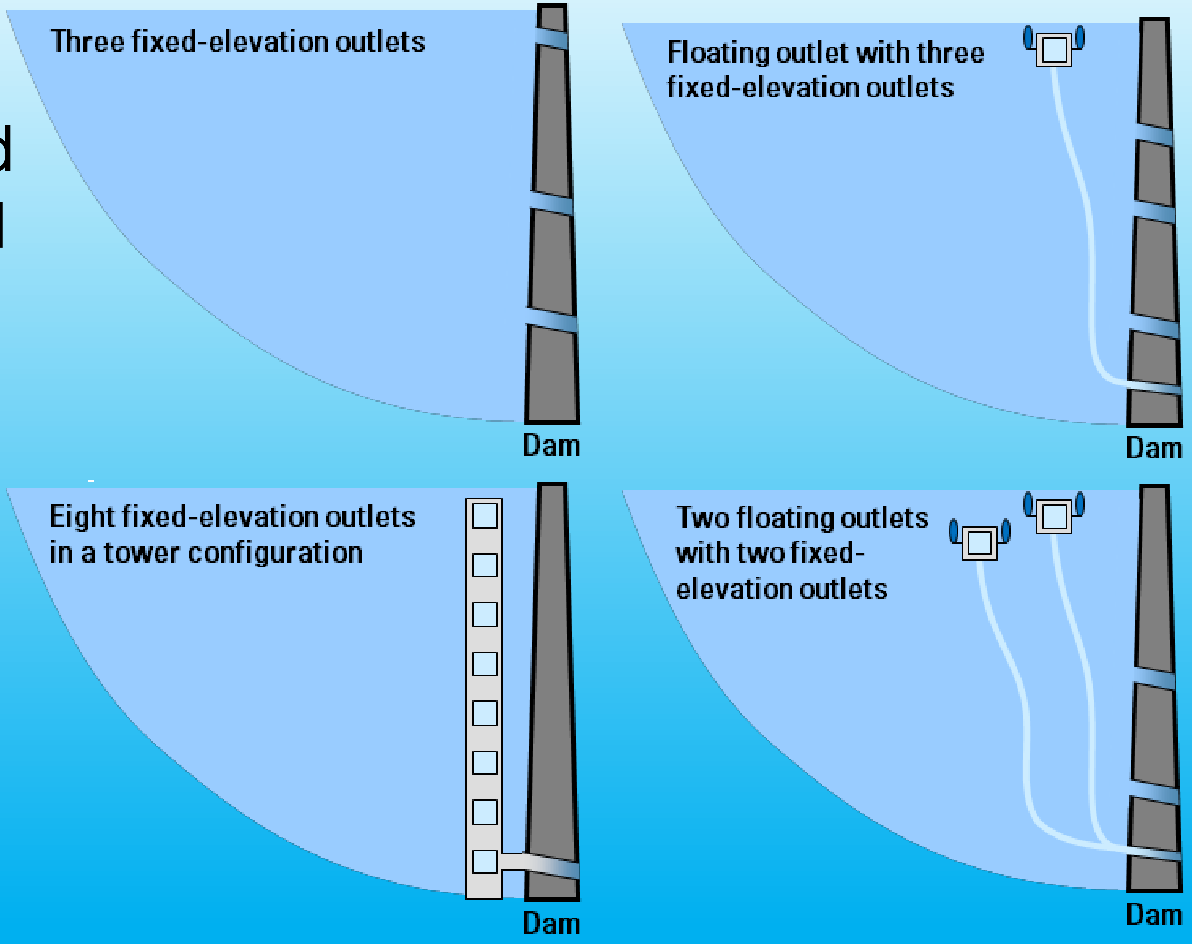




Selective Withdrawal

- Selective withdrawal facilities
- Selective withdrawal uses stratified flow to pull out water from selected depths of the pool.

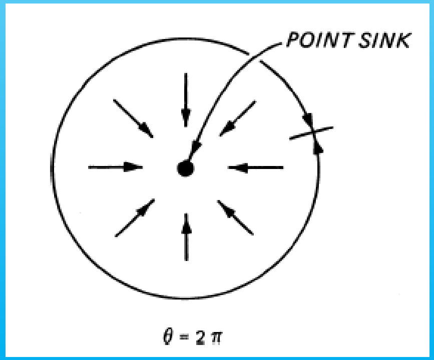


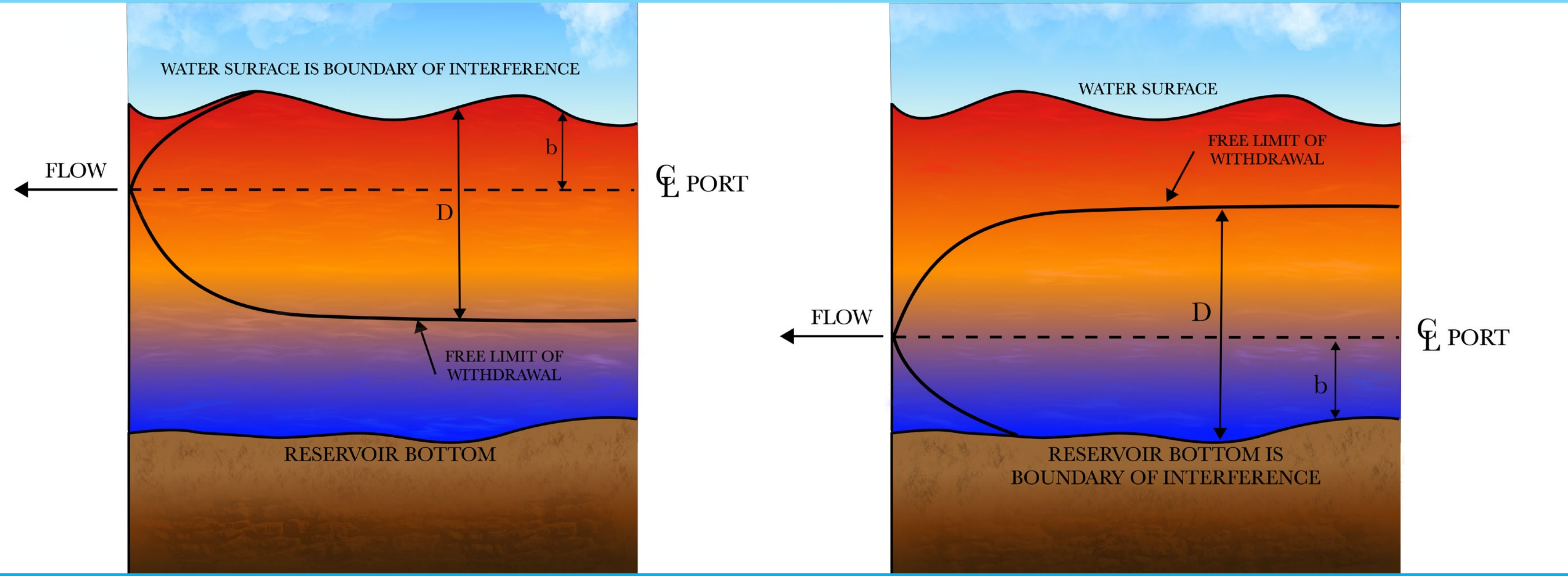


Courtesy of USGS

Selective Withdrawal

- Selective withdrawal algorithm determines the vertical zone limits based on the outflow, outlet geometry and in-pool densities
  - A horizontal withdrawal angle is included (Bohan and Grace,1973)
  - Boundary interference is included into the calculations of the withdrawal zone limits

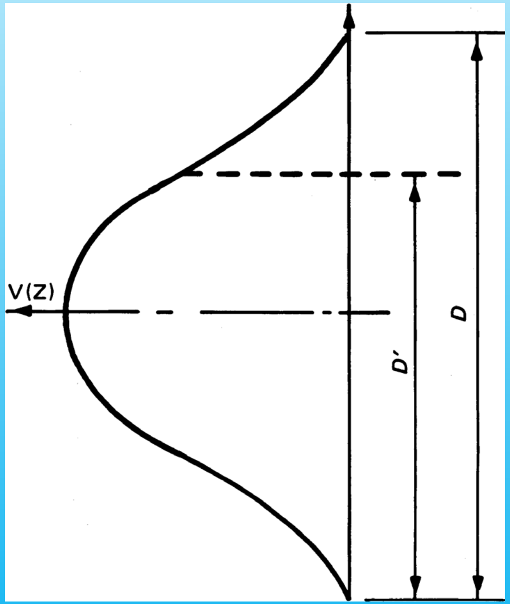


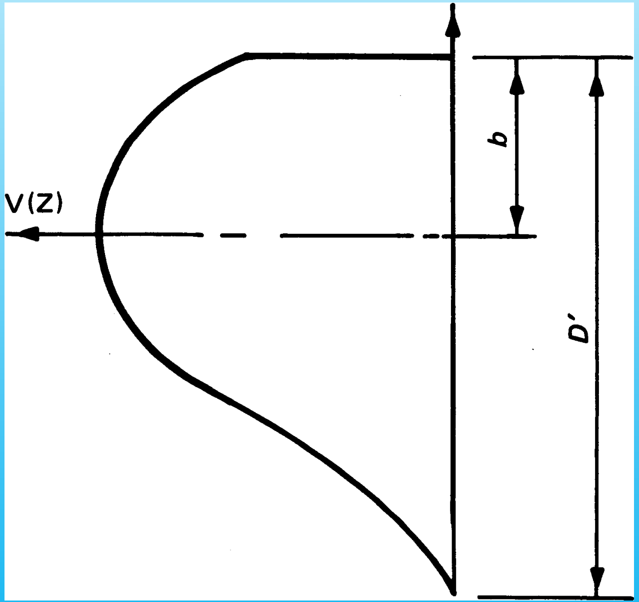


Graphics by Lauren Melendez

Selective Withdrawal

- Update calculation of withdrawal zone profile and limits





$$\frac{Q}{D'^3 N} - \frac{0.125\phi}{X^3}\frac{}{\theta\pi} = 0$$

$$\phi = \frac{1}{2}\left[1 + \frac{1}{\pi}\sin\left(\frac{\frac{b}{D'}}{1-\frac{b}{D'}}\pi\right) + \frac{\frac{b}{D'}}{1-\frac{b}{D'}}\right]$$

$$X = \frac{1}{2}\left[1 + \frac{\frac{b}{D'}}{1-\frac{b}{D'}}\right]$$

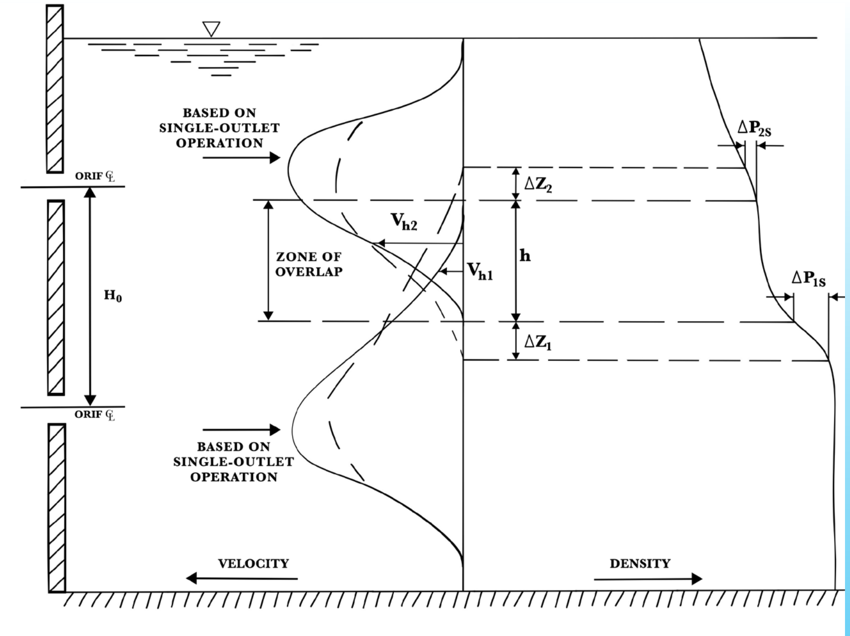
Selective Withdrawal

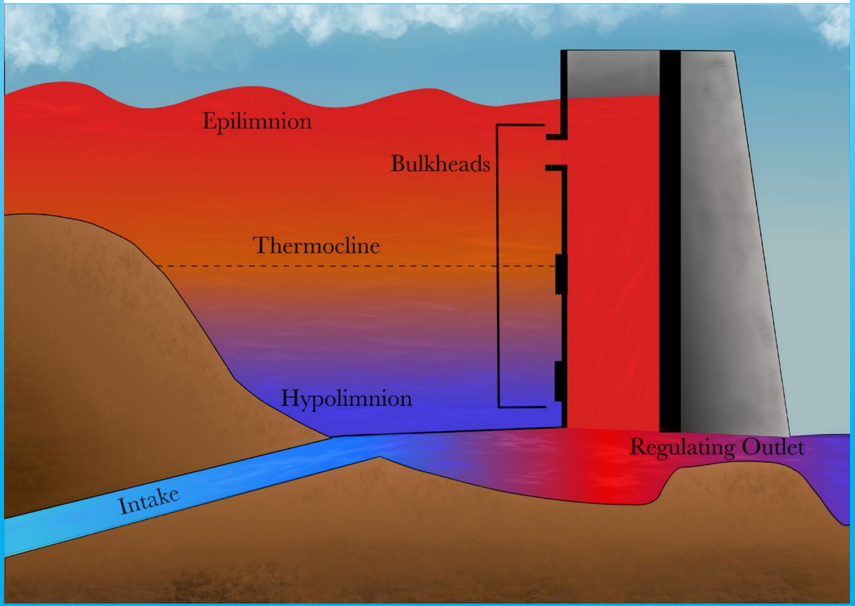
- Update the calculation of the Velocity Profile for overlapping withdrawal zones:

$$v_k = \left(1 - \frac{y_i}{Y_1}\frac{\square}{\square \quad m}\right)^2$$

- Calculate flow distribution and outflow for simultaneous, multi-level withdrawal (Howington, 1990):

$$Q_i = \sqrt{\frac{2gA_i^2}{k_i}HL_i}$$





Graphics by Lauren Melendez

Selective Withdrawal

Additional inputs for withdrawal structures

STRUCTURES for each branch. These are known outflows at the end of a branch	BR1	BR2
NSTR - Number of branch outlet structures	4	
DYNSTRUC - Dynamic elevation of structure control ON or OFF - reads input file	OFF	
STRIC1-Turns ON/OFF interpolation of structure outflows for structure 1	ON	
STRIC2-Turns ON/OFF interpolation of structure outflows for structure 2	ON	
STRIC3-Turns ON/OFF interpolation of structure outflows for structure 3	ON	
STRIC4-Turns ON/OFF interpolation of structure outflows for structure 4	ON	
STRIC5-Turns ON/OFF interpolation of structure outflows for structure 5		
KTSTR1-Top layer above which selective withdrawal will not occur for structure 1	2	
KTSTR2-Top layer above which selective withdrawal will not occur for structure 2	2	
KTSTR3-Top layer above which selective withdrawal will not occur for structure 3	2	
KTSTR4-Top layer above which selective withdrawal will not occur for structure 4	2	
KTSTR5-Top layer above which selective withdrawal will not occur for structure 5		
KBSTR1-Bottom layer below which selective withdrawal will not occur for structure 1	35	
KBSTR2-Bottom layer below which selective withdrawal will not occur for structure 2	35	
KBSTR3-Bottom layer below which selective withdrawal will not occur for structure 3	35	
KBSTR4-Bottom layer below which selective withdrawal will not occur for structure 4	35	
KBSTR5-Bottom layer below which selective withdrawal will not occur for structure 5		
SINKC1 - Sink type used in the selective withdrawal algorithm, LINE or POINT, structure 1	POINT	
SINKC2 - Sink type used in the selective withdrawal algorithm, LINE or POINT, structure 2	POINT	
SINKC3 - Sink type used in the selective withdrawal algorithm, LINE or POINT, structure 3	POINT	
SINKC4 - Sink type used in the selective withdrawal algorithm, LINE or POINT, structure 4	POINT	
SINKC5 - Sink type used in the selective withdrawal algorithm, LINE or POINT, structure 5		
ESTR1-Centerline elevation of structure 1, m	104	
ESTR2-Centerline elevation of structure 2, m	110	
ESTR3-Centerline elevation of structure 3, m	107	
ESTR4-Centerline elevation of structure 4, m	72	
ESTR5-Centerline elevation of structure 5, m		
WSTR1 - Structure 1 width if "LINE" chosen, Width of structure (line sink), m	0	
WSTR2- Structure 2 width if "LINE" chosen, Width of structure (line sink), m	0	
WSTR3- Structure 3 width if "LINE" chosen, Width of structure (line sink), m	0	
WSTR4- Structure 4 width if "LINE" chosen, Width of structure (line sink), m	0	
WSTR5- Structure 5 width if "LINE" chosen, Width of structure (line sink), m		
Theta_STRT1 - Structure 1 Effective Angle of Withdrawal, radians	3.14	
Theta_STRT2 - Structure 2 Effective Angle of Withdrawal, radians	3.14	
Theta_STRT3 - Structure 3 Effective Angle of Withdrawal, radians	3.14	
Theta_STRT4 - Structure 4 Effective Angle of Withdrawal, radians	3.14	
Theta_STRT5 - Structure 5 Effective Angle of Withdrawal, radians		

CE-QUAL-W2 Input Files

w2_con.xlsm – develops W2 control files

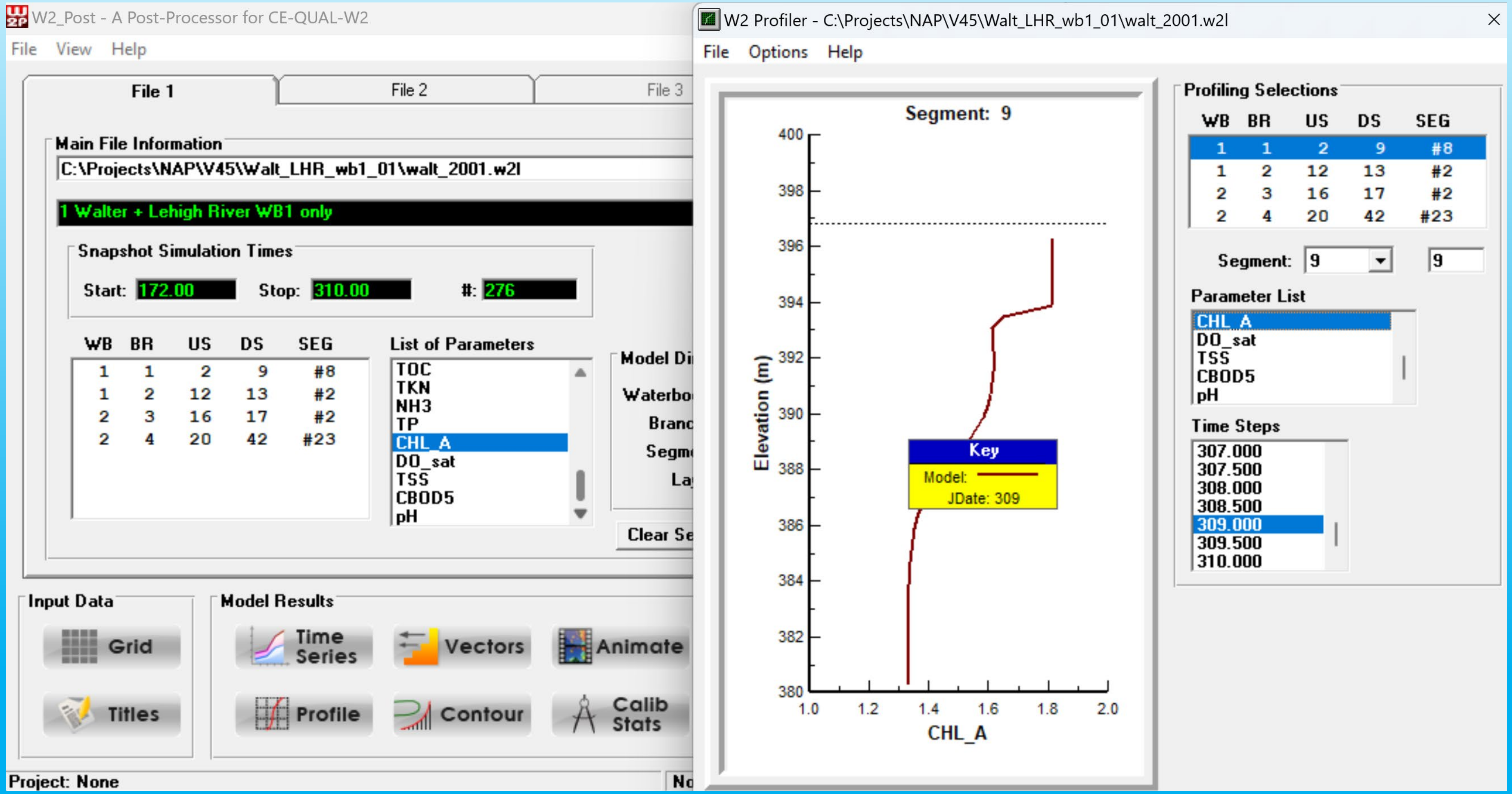
NWB	NBR	IMX	KMX	NPROC	CLOSEC						
5	7	239	102	1	OFF						
NTR	NST	NIW	NWD	NGT	NSP	NPI	NPU				
2	0	0	0	6	0	0	0				
NGC	NSS	NAL	NEP	NBOD	NMC	NZP					
3	2	3	1	0	0	1					
NDAY	SELECTC	HABTATC	ENVIRPC	AERATEC	INITUWL	ORGCC	SED_DIAG	HG	ISSON	DZMAX	HDF5
400	OFF	ON	OFF	OFF	OFF	OFF	ON	ON	ON	100	
TMSTRT	TMEND	YEAR									
1.000	1826	2014									
NDLT	DLTMIN	DLTINTER									
9	0.01	OFF									
DLTD	DLTD	DLTD	DLTD	DLTD	DLTD	DLTD	DLTD	DLTD	DLTD	DLTD	DLTD
1	100	130	470	500	760	800	1180	1200			
DLTMAX	DLTMAX	DLTMAX	DLTMAX	DLTMAX	DLTMAX	DLTMAX	DLTMAX	DLTMAX	DLTMAX	DLTMAX	DLTMAX
60	30	60	30	60	30	60	30	60			
DLTF	DLTF	DLTF	DLTF	DLTF	DLTF	DLTF	DLTF	DLTF	DLTF	DLTF	DLTF
0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9			
WB1	WB2	WB3	WB4	WB5	WB6	WB7	WB8	WB9	WB10		
ON	ON	ON	ON	ON							
ON	ON	ON	ON	ON							

CE-QUAL-W2 Output Files

- Water body: flow balance file, N and P mass balance file, water level file, flux file
- Outlet hydraulic structure output files
- W2L file for W2_Post
- HDF5 file
- Additional outputs

CE-QUAL-W2 Output Files

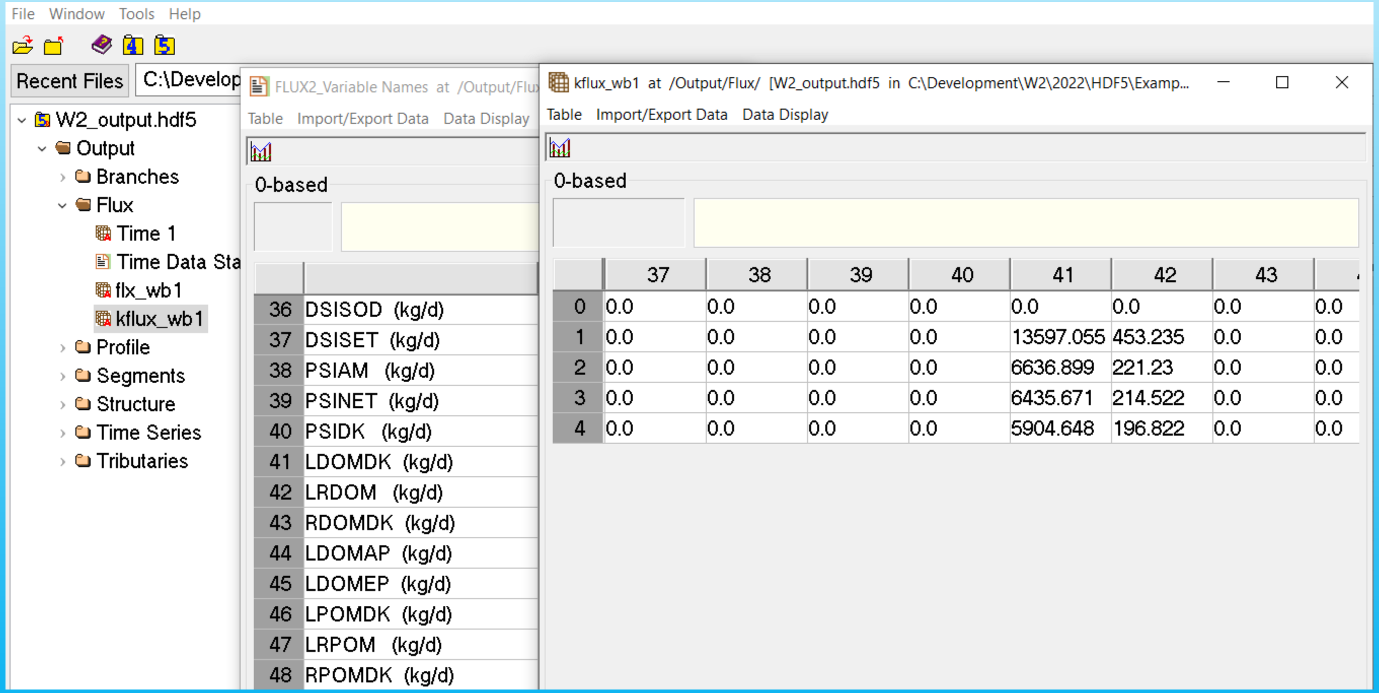
W2L – includes derived variables



CE-QUAL-W2 Output Files

HDF5 – includes model outputs in table format

1. Kinetic Flux (KFL)
2. Profile (PRF)
3. Time Series (TSR)
4. Branches
5. Segments
6. Hydraulic Structures
7. Tributaries



Questions?