OVERVIEW OF CE-QUAL-W2 VERSION 4.5

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CE-QUAL-W2 Workshop

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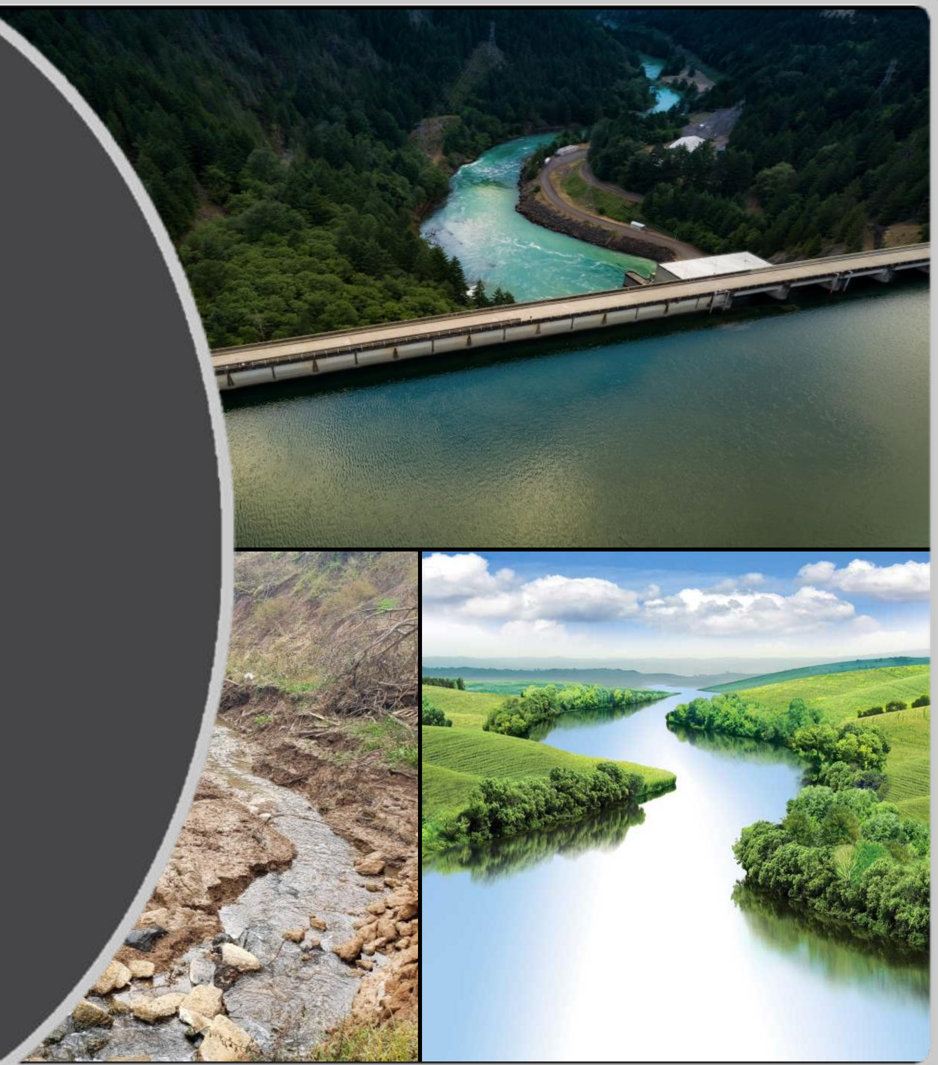


Outline

1. W2 version 4.5 inputs/outputs

2. Water quality kinetics
   - State variables
   - Derived variables
   - WQ processes
   - TDG/SYSTDG
   - Bed sediment

3. V4.5 tools

CE-QUAL-W2 V4.5 Inputs

- Control file changes
  - ▸csv format
  - ▸Excel template to support develop input control files
  - ▸Excel file w2_con.xlsm → w2_con.csv
- Time series file changes - csv format
- Atmospheric deposition inputs of WQ state variables
- Atmospheric CO_2 input changes
- Oxygen reaeration

w2_con.csv!A1
Required Constituent Order'!A1
w2_habitat.npt!A1
w2_aerate.npt!A1
w2_envirprf.npt!A1
w2_selective.npt!A1
w2_constriction.csv!A1
w2_particle.csv!A1
w2_multiple_WB.npt!A1
w2_tecplotbr.csv!A1
w2_systdg.npt!A1
w2_TDGTarget.csv!A1
w2_lake_river_contour.csv!A1
w2_AlgaeMigration.csv!A1
w2_Algae_Toxin.csv!A1
w2_diagenesis.npt!A1

CE-QUAL-W2 Control File: w2_con.xlsm

Export to CSV file

8	NBR: number of branches		"Default light absorption/extinction coefficients"							
9	IMX: maximum number of segments including inactive segmen		"Testing sensitivity of temperature predictions to vertical resolution"							
10	KMX: maximum number of vertical layers including inactive lay		"2 m layer heights"							
11	NPROC: # of processors (INACTIVE at this time)		"Atmosperic Deposition Feature"							
12	CLOSEC: close dialog box after executing if =ON		""							
13	NTR: number of tributaries		""							
14	NST: maximum # of	structures in a branch								
15	NIW: # of internal w	**GRID/NPROC/CLOSE DIALOG BOX**	**NWB**	NBR	IMX	KMX	NPROC	CLOSEC		
16	NWD: # of withdrawals		1	1	32	36	1	OFF		
17	NGT: # of gates									
18	NSP: # of spillways	**IN/OUTFLOW**	**NTR**	NST	NIW	NWD	NGT	NSP	NPI	NPU
19	NPI: # of pipes		0	1	0	0	1	0	0	0
20	NPU: # of pumps or	water level control rules								
21	NGC: # of generic w	**CONSTITUENTS**	**NGC**	NSS	NAL	NEP	NBOD	NMC	NZP	
22	**Do not change bolded headers in COL C - these are checked by the program**		3	1	1	1	0	0	1	
23	NDAY:Maximum number of output dates or timestep related changes									
24	SELECTC:Turn ON/OF	**MISCELLANEOUS**	**NDAY**	SELECTC	HABTATC	ENVIRPC	AERATEC	INITUWL	ORGCC	SED_DIAG
25	HABITATC:Turn ON/OFF habitat analyses for fish and eutrophication variables		100	ON	ON	ON	ON	OFF	OFF	ON
26	ENVIRPC:Turn ON/OFF environmental performance criteria									
27	AERATEC:Turn ON/OI	**TIME CON**	**TMSTRT**	TMEND	YEAR					
28	INITUWL:Turn ON/OI	These are computed from formula in Column A-->	64.500	358.7	1980					
29	ORGCC simulates the	organic matter as C rather than organic matter; SED_DIAG: turns ON/								
30	**Fill in these with rea**	**DLT CON**	**NDLT**	DLTMIN	DLTINTER					
31	**TMSTRT**	Time step control parameters	1	1	OFF					
32	**3/4/1980 12:00**									
33	**TMEND**	**DLT DATE**	DLTD	DLTD	DLTD	DLTD	DLTD	DLTD	DLTD	DLTD
34	**12/23/1980 16:48**	Date of time step change in JDAY	64.5							

w2_con.csv | Required Constituent Order | w2_habitat.npt | w2_diagenesis.npt | w2_ ...

CE-QUAL-W2 Control File: w2_con.xlsm

NST: maximum # of structures in a branch					
NIW: # of internal weirs	GRID/NPROC/CLOSE DIALOG BOX	**NWB**	NBR	IMX	KI
NWD: # of withdrawals		1	1	32	
NGT: # of gates					
NSP: # of spillways	IN/OUTFLOW	**NTR**	NST	NIW	N
NPI: # of pipes		0	1	0	
NPU: # of pumps or water level control rules					
NGC: # of generic water quality constituents	CONSTITUENTS	**NGC**	NSS	NAL	NI
Do not change bolded headers in COL C - these are checked by the program		3	1	1	
NDAY:Maximum number of output dates or timestep related changes					
SELECTC:Turn ON/OFF/USGS automatic port selection from a multiple outlet s	MISCELLANEOUS	**NDAY**	SELECTC	HABTATC	EN
HABTATC:Turn ON/OFF habitat analyses for fish and eutrophication variables		100	ON	ON	OI
ENVIRPC:Turn ON/OFF environmental performance criteria					
AERATEC:Turn ON/OFF aeration to waterbody with dissolved oxygen probe co	TIME CON	**TMSTRT**	TMEND	YEAR	
INITUWL:Turn ON/OFF initial water surface slope and velocity calculation for	These are computed from formula in Column A-->	64.500	358.7	1980	
Fill in these with real dates and the Julian dates will be filled in automatically	DLT CON	**NDLT**	DLTMIN	DLTINTER	
TMSTRT	Time step control parameters	1	1	OFF	
3/4/1980 12:00					
TMEND	DLT DATE	DLTD	DLTD	DLTD	DL
12/23/1980 16:48	Date of time step change in JDAY	64.5			

CE-QUAL-W2 Control File: w2_con.xlsm

A	B	C	D	E	F	G	H	I	J	K	L	M	N
CO2YRLY:CO2YearlyGlobalAverage ON or OFF, use global yearly average CO2 based on regression eqn													
	ATMOSPHERIC DEPOSITION	WB1	WB2	WB3	WB4	WB5	WB6	WB7	WB8	WB9	WB10		
	Atm_DepositionC - turn ON/OFF mass loading (kg/km2/year) for each water body	ON											
	Atm_Deposition_Interpolation - Interpolate between values ON/OFF	ON											
Verify that you have this many constituent rows below:	**28**						Repeat columns as necessary - EVEN IF NO TRIBUTARIES INCLUDE A COLUMN FOR CTRTRC1 (It can be blanks						
	CST - Concentration State variables and initial conditions	CNAME2 Short na	CNAME Long name	CAC Active	FMTC Fort	CMULT Output N	C2IWB1 Initial cor	CPRWBC1	C_Atm_Depositon	CINBRC1 I	CTRTRC1 T	CDTBRC1	CPRBRC1 Precipitation c
Must include text in quotes if there are spaces or other symbols like '/' for C	1	TDS	"TDS, g/m^3	ON	(f10.3)	1	51	ON	OFF	ON	OFF	OFF	OFF
SEE TAB SHOWING REQUIRED CONSTITUENT ORDER	2	Gen1	"GC1, g/m^3	ON	(f10.3)	1	100	ON	OFF	ON	OFF	OFF	OFF
	3	Gen2	"Age, days	ON	(f10.3)	1	0	OFF	OFF	OFF	OFF	OFF	OFF
Note that epiphyton and macrophytes are turned ON below, not here	4	Gen3	"GC3, g/m^3	ON	(f10.3)	1	10	OFF	OFF	ON	OFF	OFF	OFF
	5	TSS1	"TSS, g/m^3	ON	(f10.3)	1	2	ON	OFF	ON	OFF	OFF	OFF
	6	PO4	"Phosphate, g/m^3	ON	(f10.3)	1	0.01	ON	ON	ON	OFF	OFF	OFF
Note the order of these columns for this section:	7	NH4	"Ammonium, g/m^	ON	(f10.3)	1	0.14	ON	ON	ON	OFF	OFF	OFF
CNAME2, CNAME, CAC, FMTC, CMULT,	8	NO3	"Nitrate-Nitrite, g/	ON	(f10.3)	1	0.14	ON	ON	ON	OFF	OFF	OFF
C2IWB (repeat for each waterbody)	9	DSI	"Dissolved silica,	OFF	(f10.3)	1	0	OFF	OFF	OFF	OFF	OFF	OFF
CPRWBC (repeat for each waterbody)	10	PSI	"Particulate silica	OFF	(f10.3)	1	0	OFF	OFF	OFF	OFF	OFF	OFF
C_Atm_Deposition (repeat for each waterbody)	11	FE	"Total iron, g/m^3	ON	(f10.3)	1	0.1	ON	OFF	ON	OFF	OFF	OFF
CINBRC (repeat for each branch)	12	LDOM	"Labile DOM, g/m^	ON	(f10.3)	1	0.7	ON	OFF	ON	OFF	OFF	OFF
CTRTRC (repeat for each tributary - include at least 1 even if no tribs)	13	RDOM	"Refractory DOM,	ON	(f10.3)	1	2.022	ON	OFF	ON	OFF	OFF	OFF
CDTBRC (repeat for each branch)	14	LPOM	"Labile POM, g/m^	ON	(f10.3)	1	0.1	ON	OFF	ON	OFF	OFF	OFF
CPRBRC (repeat for each branch)	15	RPOM	"Refractory POM,	OFF	(f10.3)	1	0	OFF	OFF	OFF	OFF	OFF	OFF
Your last column should be in COLUMN:	16	ALG1	"Algae, g/m^3	ON	(f10.3)	1	-1	ON	OFF	ON	OFF	OFF	OFF
N	17	DO	"Dissolved oxygen	ON	(f10.3)	1	-1	ON	OFF	ON	OFF	OFF	OFF
12	18	TIC	"Inorganic carbon	ON	(f10.3)	1	11.91	OFF	OFF	ON	OFF	OFF	OFF
	19	ALK	"Alkalinity, g/m^3	ON	(f10.3)	1	31	OFF	OFF	ON	OFF	OFF	OFF
	20	ZOO1	"zooplankton1, mg	OFF	(g10.3)	1	0.1	OFF	OFF	OFF	OFF	OFF	OFF
	21	LDOM_P	"LDOM P, mg/m^3	OFF	(g10.3)	1	0.0005	OFF	OFF	OFF	OFF	OFF	OFF
	22	RDOM_P	"RDOM P, mg/m^3	OFF	(g10.3)	1	0.0005	OFF	OFF	OFF	OFF	OFF	OFF
	23	LPOM_P	"LPOM P, mg/m^3	OFF	(g10.3)	1	0.0005	OFF	ON	OFF	OFF	OFF	OFF
	24	RPOM_P	"RPOM P, mg/m^3	OFF	(g10.3)	1	0.0005	OFF	ON	OFF	OFF	OFF	OFF
	25	LDOM_N	"LDOM N, mg/m^3	OFF	(g10.3)	1	0.008	OFF	OFF	OFF	OFF	OFF	OFF
	26	RDOM_N	"RDOM N, mg/m^3	OFF	(g10.3)	1	0.008	OFF	OFF	OFF	OFF	OFF	OFF
	27	LPOM_N	"LPOM N, mg/m^3	OFF	(g10.3)	1	0.008	OFF	OFF	OFF	OFF	OFF	OFF
	28	RPOM_N	"RPOM N, mg/m^3	OFF	(g10.3)	1	0.008	OFF	OFF	OFF	OFF	OFF	OFF

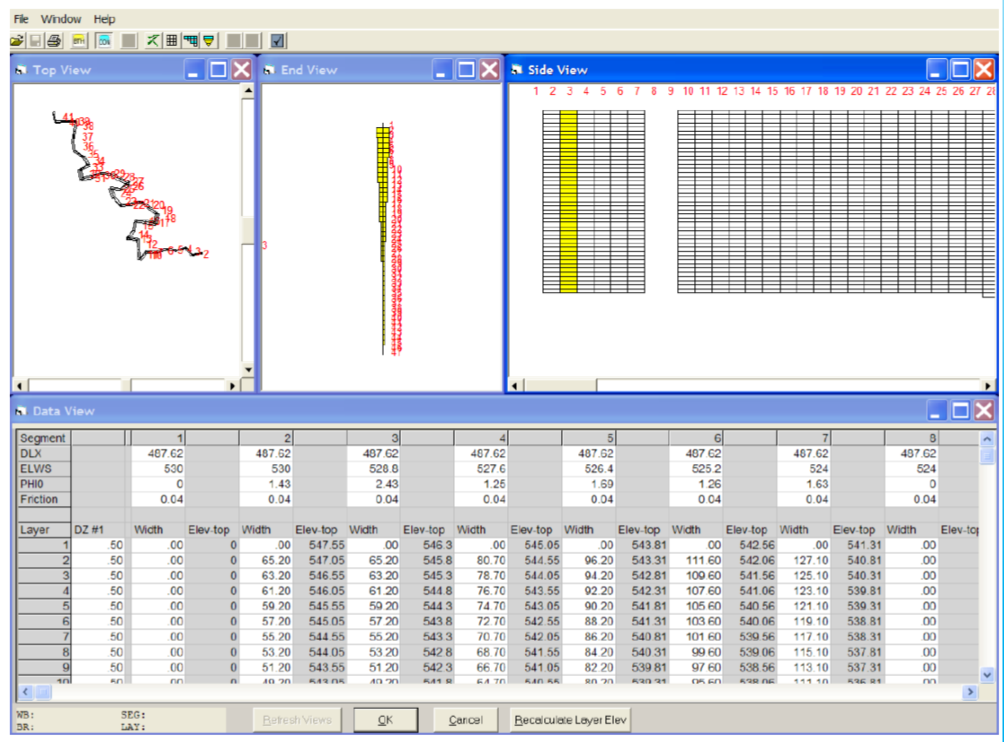
CE-QUAL-W2 Control File: w2_con.xlsm

Advantages

- Simplified editing
- No graph.npt
- Easier for cutting and pasting
- Simplified I/O
- Files are better organized
- Variable names and explanations at your fingertips
- Formulae are used to assist in control file development

Disadvantages

- Macro – Security
- W2 GUI Interface (W2_Control) for Versions 3.7-4.2 is broken

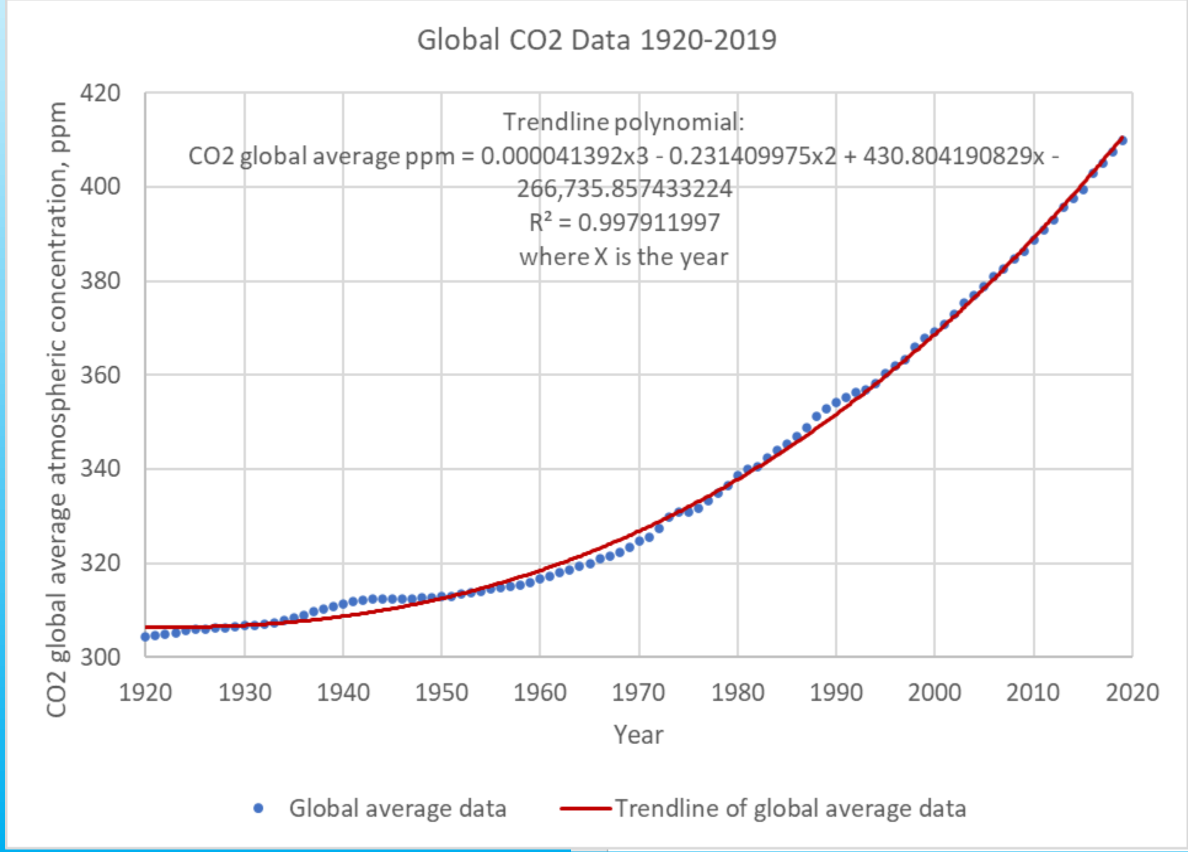


Atmospheric Deposition Inputs of WQ State Variables

- Atmospheric deposition: either dry or wet deposition (rain or snow) of pollutants contribute to the mass loading of a pollutant.
- Dry deposition can include dust or particle transport associated with the pollutant.
- The processes of atmospheric deposition include any state variables in W2.

$atm_deposition_wb1.csv					
Atmospheric mass input, kg/km2/year					
JDAY	PO4	NH4	NO3	LPOMP	RPOMP
1	14	0.6	2	1	1
100	16	0.7	2	1	1
250	18	0.6	2	1	1
365	14	0.7	2	1	1
400	14	0.6	2	1	1

Atmospheric CO2 Input Changes



DO CBOD uptake - sink, kg/day	DOCBOD	OFF	
DO reaeration - source/sink, kg/day	DOREAR	ON	
DO sediment uptake - sink, kg/day	DOSED	ON	
DO SOD uptake - sink, kg/day	DOSOD	OFF	
TIC algal uptake - sink, kg/day	TICAG	OFF	
TIC epiphyton uptake - sink, kg/day	TICEG	OFF	
Sediment decay - sink, kg/day	SEDDK	OFF	
Sediment algal settling - sink, kg/day	SEDAS	OFF	
Sediment LPOM settling - source,kg/day	SEDLPOM	OFF	
Sediment net settling - source/sink, kg/day	SEDSET	OFF	
SOD decay - sink, kg/day	SODDK	OFF	
CO2 ATMOSPHERIC CONC			
CO2inAtmospherePPM, CO2 atmospheric concentration in ppm CO2	405		
CO2YearlyGlobalAverage ON or OFF, use global yearly average CO2 based on regres	ON		
EX COEF	WB1	WB2	WB3
EXH2O - water light extinction- 1/m	0.45		
EXSS - suspended solids light extinction- 1/m	0.01		
EXOM - extinction organic matter- 1/(m mg/l)	0.2		
BETA - fraction short wave absorbed on surface	0.45		
EXC - Read in light extinction time series ON or OFF	OFF		
EXIC - Interpolation of light extinction time series ON or OFF	OFF		
ALG EXTINCTION	EXA1	EXA2	EXA3
Algae light extinction- 1/(m mg/l)	0.2		
ZOO EXTINCTION	EXZ1	EXZ2	EXZ3
Zooplankton light extinction- 1/(m mg/l)	0.2		

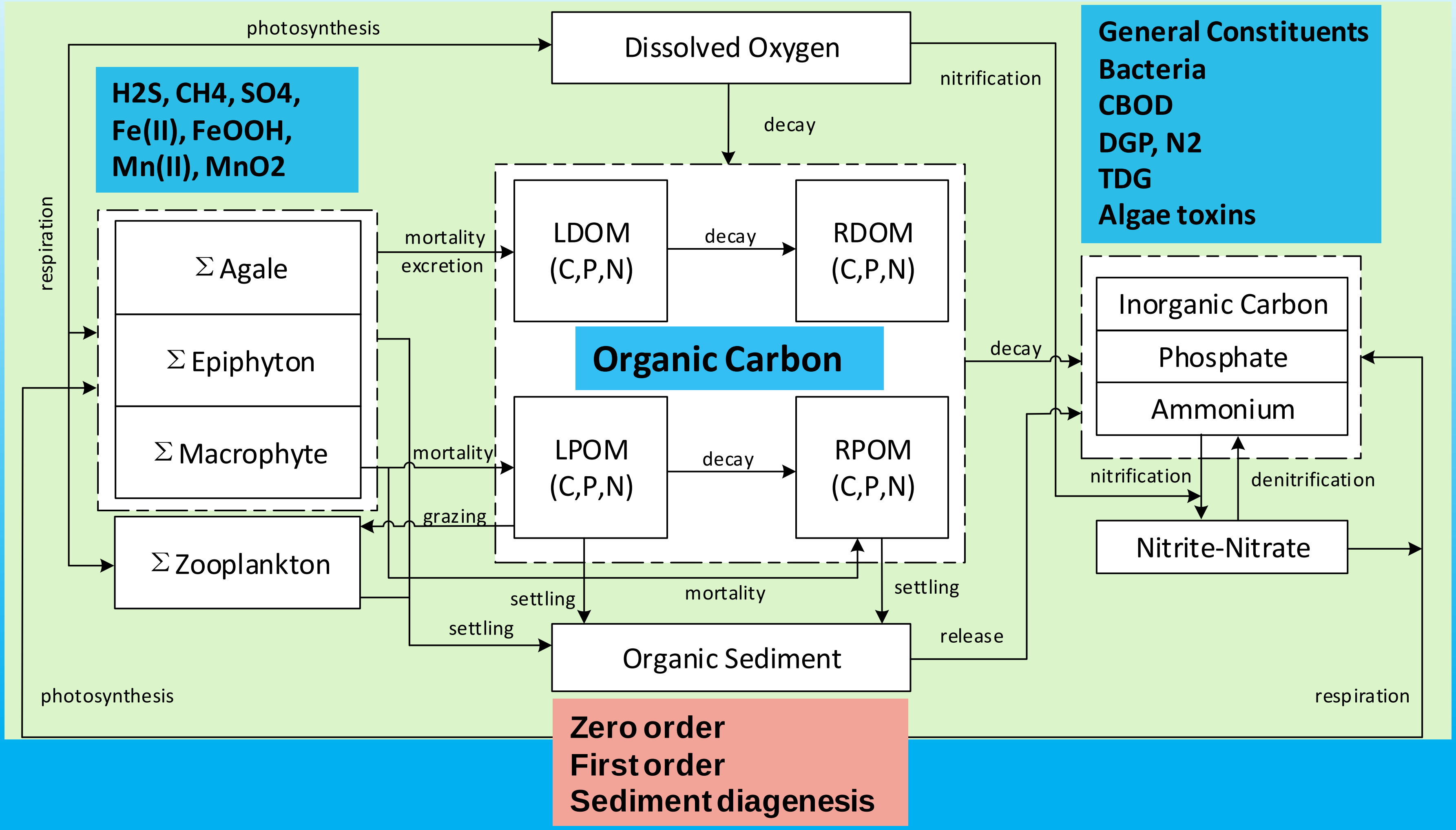
Additional Outputs

- Mass balance of TN and TP
- Water body fluxes of 72 pathways
- Selective withdrawal outputs in snapshot (*.snp) file
- Contour plots
  - Ability to generate lake contours easily (elevation vs time for temperature and DO)
  - Ability to generate river contours easily (model segment or distance along river vs time for temperature and DO)

Water Quality Kinetics

- State variables
  - New state variables: Water age, Bacteria, **DGP, N2, H2S, CH4, SO4, Fe species (FEII, FEOOH), Mn species (MnII, MnO2)**
- Directly simulates organic carbon constituents (**LDOC, RDOC, LPOC, RPOC**)
- Algae toxins
- New derived variables: Turbidity, Secchi disk, TDG, NH3
- Sediment Diagenesis updates: control file, computation efficiency
- Vertical migration of zooplankton and cyanobacteria

Water Quality Kinetics



Water Quality State Variables

- TDS
- Gen1
- Gen2
- ISS1
- ISS2
- WaterAge
- Bacteria
- DGP
- N2
- H2S
- CH4
- SO4
- Fe (II)
- FeOOH
- Mn (II)
- MnO2

- PO4
- NH4
- NO3
- DSI
- PSI
- LDOM (LDOC)
- RDOM (RDOC)
- LPOM (LPOC)
- RPOM (RPOC)
- CBOD1
- CBODP1
- CBODN1
- ALG1
- ALG2
- DO
- TIC

- ALK
- LDOM-P
- RDOM-P
- LPOM-P
- RPOM-P
- LDOM-N
- RDOM-N
- LPOM-N
- RPOM-N
- MICROSYSTIN
- CYLINDROSPERMOPSIN
- ANATOXIN-A
- SAXITOXIN

	CNAME2 Short na	CNAME Long name	CAC Active	FMTC Fortr	CMULT Output M
1	TDS	"TDS, g/m^3	ON	(f10.3)	1
2	Gen1	"GC1, g/m^3	ON	(f10.3)	1
3	Gen2	"GC2, g/m3	OFF	(f10.3)	1
4	Gen3	"GC3, g/m^3	ON	(f10.3)	1
5	ISS1	"ISS, g/m^3	ON	(f10.3)	1
6	WaterAge	"Age, days"	OFF	(f10.3)	1
7	Bacteria	"Bacteria, col/100	OFF	(f10.3)	1
8	DGP	"Dissolved Gas Pre	OFF	(f10.3)	1
9	N2	"N2 dissolved gas,	ON	(f10.3)	1
10	H2S	"H2S, dissolved ga	OFF	(f10.3)	1
11	CH4	"CH4 dissolved ga	OFF	(f10.3)	1
12	SO4	"SO4 dissolved, m	OFF	(f10.3)	1
13	FEII	"Reduced FE(II), m	OFF	(f10.3)	1
14	FEOOH	"Oxidized FeOOH,	OFF	(f10.3)	1
15	MnII	"Reduced Mn(II),	OFF	(f10.3)	1
16	MnO2	"Oxidized MnO2,	OFF	(f10.3)	1
17	PO4	"Phosphate, g/m^	ON	(f10.3)	1
18	NH4	"Ammonium, g/m	ON	(f10.3)	1
19	NO3	"Nitrate-Nitrite, g	ON	(f10.3)	1
20	DSI	"Dissolved silica, g	OFF	(f10.3)	1
21	PSI	"Particulate silica,	OFF	(f10.3)	1
22	LDOM	"Labile DOM, g/m	ON	(f10.3)	1
23	RDOM	"Refractory DOM,	ON	(f10.3)	1
24	LPOM	"Labile POM, g/m	ON	(f10.3)	1
25	RPOM	"Refractory POM,	OFF	(f10.3)	1
26	ALG1	"Algae, g/m^3	ON	(f10.3)	1
27	DO	"Dissolved oxyger	ON	(f10.3)	1
28	TIC	"Inorganic carbon,	ON	(f10.3)	1
29	ALK	"Alkalinity, g/m^3	ON	(f10.3)	1
30	ZOO1	"zooplankton1, m	OFF	(g10.3)	1
31	LDOM_P	"LDOM P, mg/m^3	OFF	(g10.3)	1
32	RDOM_P	"RDOM P, mg/m^3	OFF	(g10.3)	1
33	LPOM_P	"LPOM P, mg/m^3	OFF	(g10.3)	1
34	RPOM_P	"RPOM P, mg/m^3	OFF	(g10.3)	1
35	LDOM_N	"LDOM N, mg/m^3	OFF	(g10.3)	1
36	RDOM_N	"RDOM N, mg/m^3	OFF	(g10.3)	1
37	LPOM_N	"LPOM N, mg/m^3	OFF	(g10.3)	1
38	RPOM_N	"RPOM N, mg/m^3	OFF	(g10.3)	1
39	MICROCYSTIN	"Microcystin, g/m	ON	(g10.3)	1
40	CYLINDROSPERM	"Clindrospermops	OFF	(g10.3)	1
41	ANATOXIN-A	"Anatoxin-A, g/m	OFF	(g10.3)	1
42	SAXITOXIN	"Saxitoxin, g/m^3	OFF	(g10.3)	1

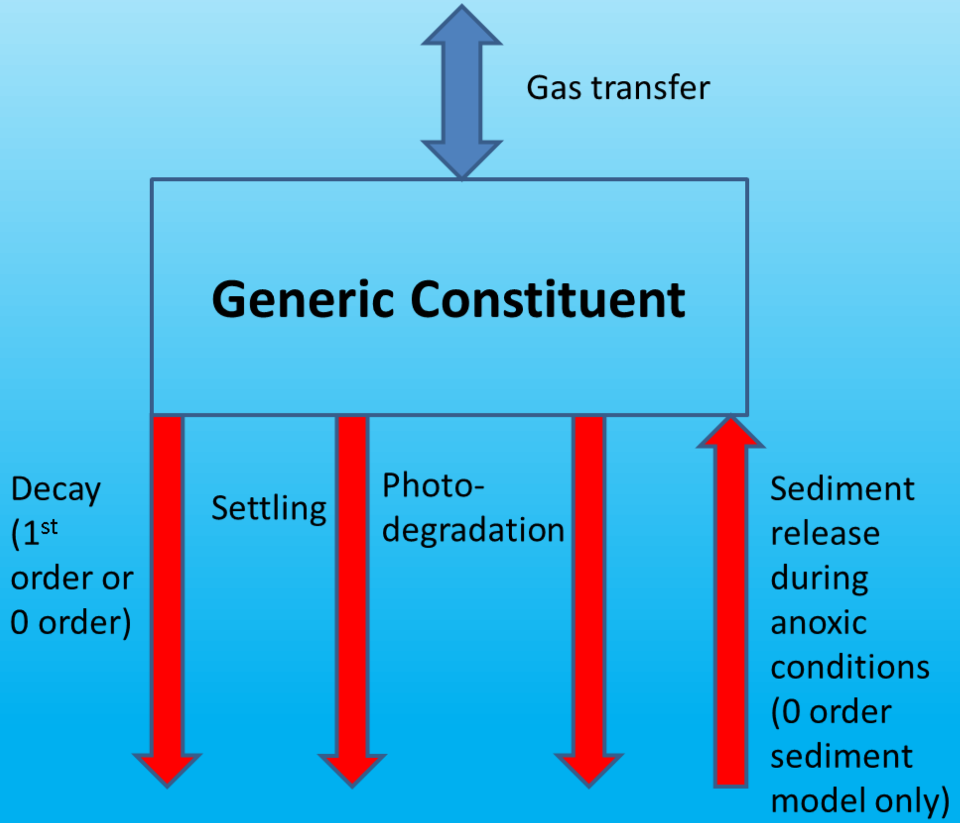
Water Quality: Derived Variables

- DOC
- POC
- TOC
- DON
- PON
- TON
- TKN
- TN
- NH3
- DOP
- POP
- TOP
- TP
- APR
- CHLA
- ATOT
- %DO
- TDG
- Turbidity
- TSS
- TISS
- CBOD
- pH
- CO2
- HCO3
- CO3
- SECCHI

CST I	CDNAME2	CDNAME	FMTCD	CDMULT
1	DOC	"Dissolved organic carbon, g/m^3 "	(F10.3)	1
2	POC	"Particulate organic carbon, g/m^3 "	(F10.3)	1
3	TOC	"Total organic carbon, g/m^3 "	(F10.3)	1
4	DON	"Dissolved organic nitrogen, g/m^3 "	(F10.3)	1
5	PON	"Particulate organic nitrogen, g/m^3 "	(F10.3)	1
6	TON	"Total organic nitrogen, g/m^3 "	(F10.3)	1
7	TKN	"Total Kheldahl Nitrogen, g/m^3 "	(F10.3)	1
8	TN	"Total nitrogen, g/m^3 "	(F10.3)	1
9	NH3	"Unionized ammonia, g/m3 as N "	(F10.3)	1
10	DOP	"Dissolved organic phosphorus, g/m^3 "	(F10.3)	1
11	POP	"Particulate organic phosphorus, g/m^3 "	(F10.3)	1
12	TOP	"Total organic phosphorus, g/m^3 "	(F10.3)	1
13	TP	"Total phosphorus, g/m^3 "	(F10.3)	1
14	APR	"Algal production, g/m^2/day "	(F10.3)	1
15	CHLA	"Chlorophyll a, mg/m^3 "	(F10.3)	1
16	ATOT	"Total algae, g/m^3 "	(F10.3)	1
17	%DO	"Oxygen % Gas Saturation "	(F10.3)	1
18	TDG	"Total dissolved gas, % "	(F10.3)	1
19	Turbidit	"Turbidity, NTU "	(F10.3)	1
20	TSS	"Total suspended Solids, g/m^3 "	(F10.3)	1
21	TISS	"Total Inorganic Suspended Solids,g/m^3 "	(F10.3)	1
22	CBOD	"Carbonaceous Ultimate BOD, g/m^3 "	(F10.3)	1
23	pH	"pH "	(F10.3)	1
24	CO2	"CO2 "	(F10.3)	1
25	HCO3	"HCO3 "	(F10.3)	1
26	CO3	"CO3 "	(F10.3)	1
27	Secchi	"Secchi disk depth, m "	(F10.3)	1

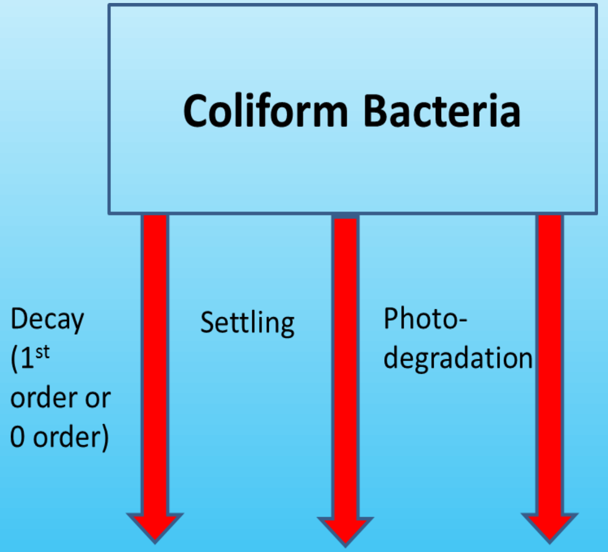
Water Quality: Generic Constituents

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



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

Water Quality: Bacteria



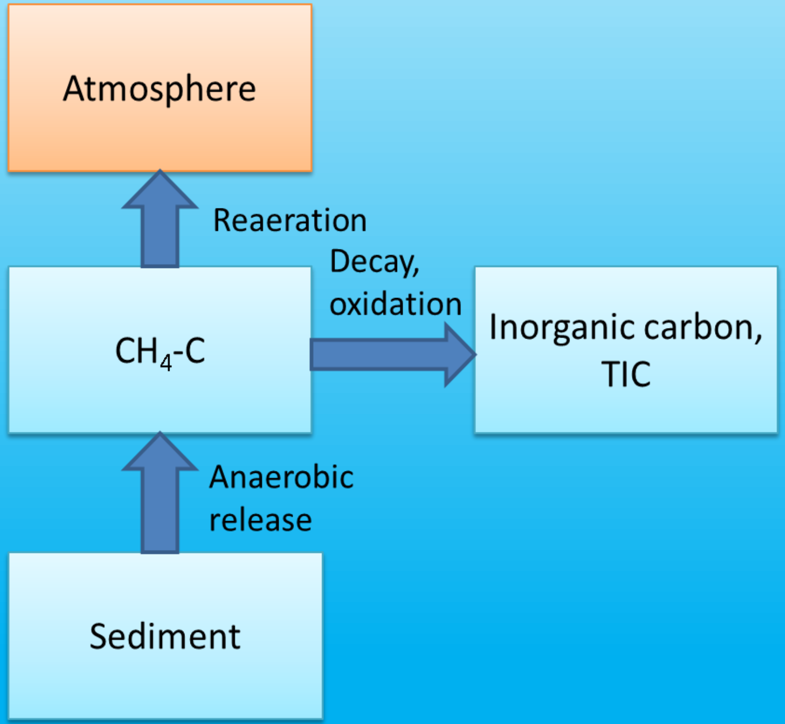
$$S_g = \underbrace{-K_{col}\,\theta^{(T\text{-}20)}\,\Phi_{col}}_{\text{1st-order decay}} - \underbrace{\omega_{col}\,\frac{\partial \Phi_{col}}{\partial z}}_{\text{settling}} - \underbrace{\alpha I_o (1-\beta) e^{-\lambda z}\,\Phi_{col}}_{\text{photodegradation}}$$

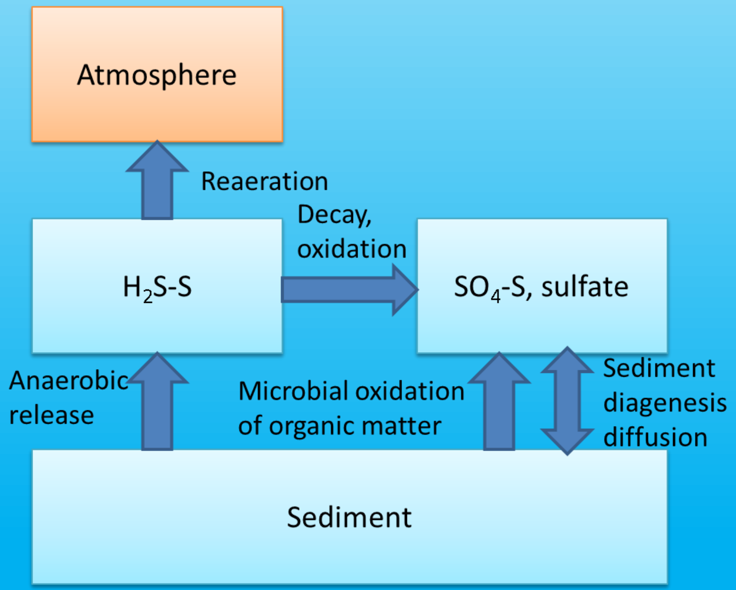
BACTERIA	WB1	WB2	W
BACTQ10, Arrhenius temperature rate multiplier, theta	1.04		
BACT1DK 1st-order decay rate, day-1	1.4		
BACTS Settling rate, m day-1	0		
BACTLDK Photodegradation parameter, m2J-1	0		

Water Quality: CH_4, H_2S

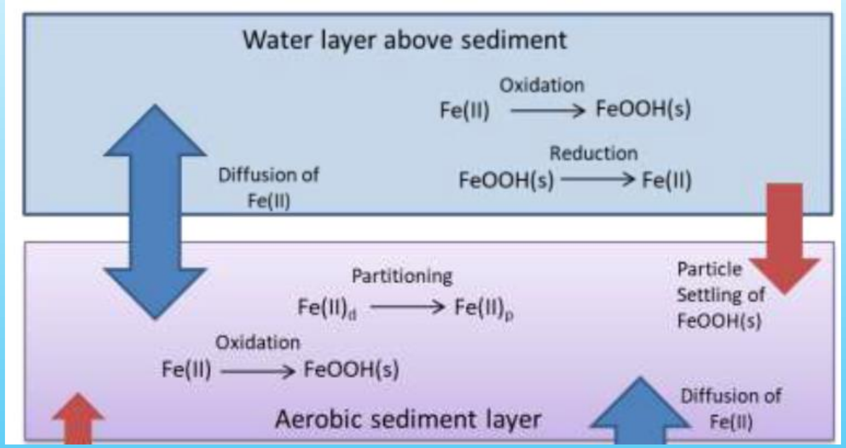
$$S = \boxed{\underbrace{SOD\,\gamma_{OM}\,\delta_{SODR}\frac{A_{sed}}{V}}_{\text{0-order sediment release}}} + \underbrace{A_{sur}K_L(-\Phi)}_{\text{reaeration}} - \underbrace{\Theta^{T-20}K\,\Phi_C}_{\text{decay}}$$

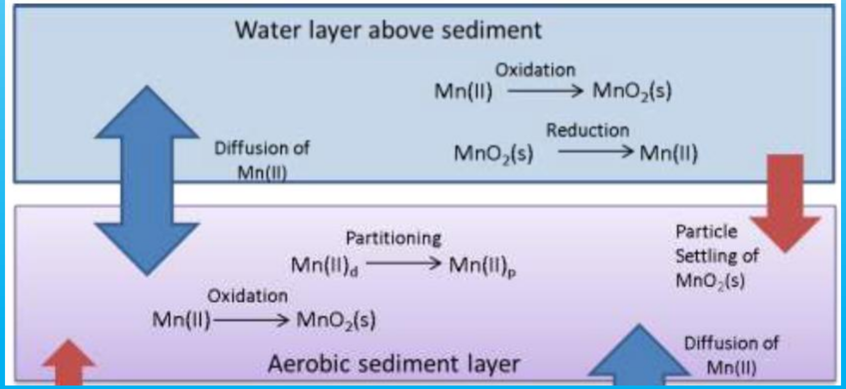
H2S	WB1
H2SR, sediment release rate, fraction of SOD (zero order),[-]	0.01
H2SQ10, Arrhenius temperature rate multiplier, theta	1.04
H2S1DK, first order decay rate, day-1	0.001
SO4R, sediment release of SO4, source, fraction of SOD (zero order), [-]	0.001
CH4	WB1
CH4R, methane sediment release rate,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





Water Quality: Fe(II), FeOOH, Mn(II), MnO_2



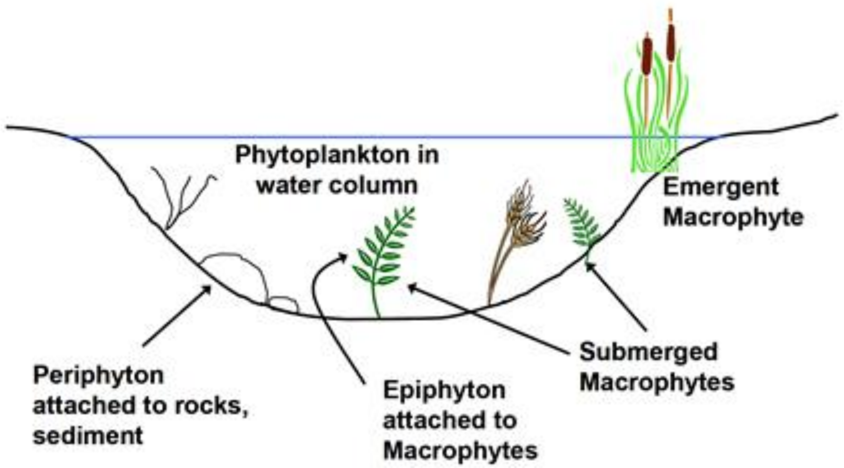


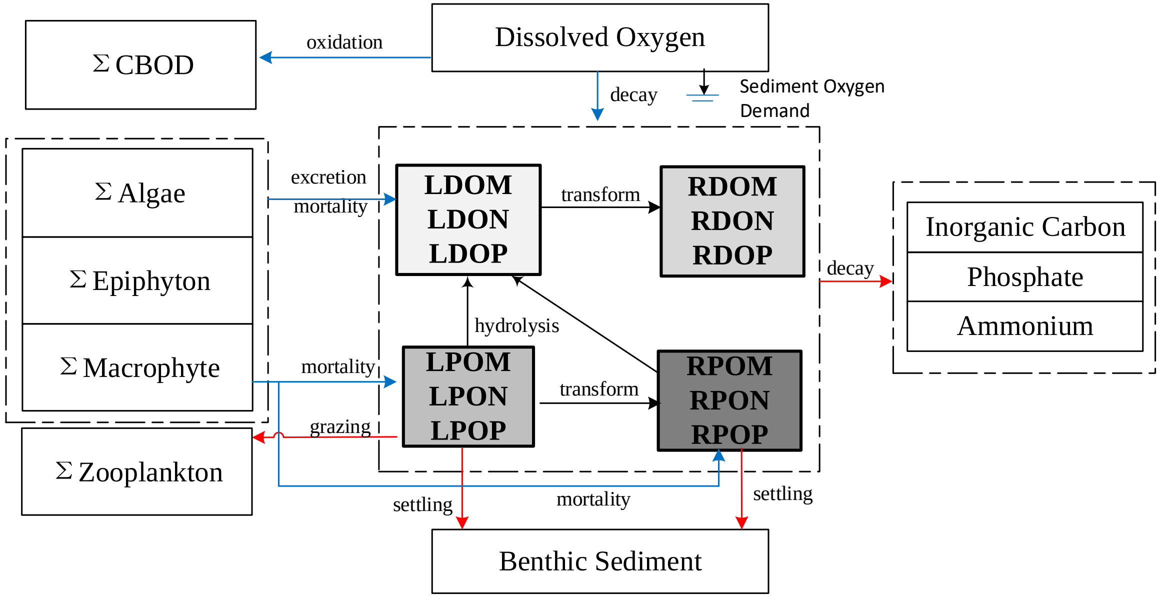
$$S_{MnII} = -K_{Mn}\Phi_{DO}\theta^{(PH-7)}\Phi_{MnII} + K_{MnO2}\frac{K_{MnO2}}{K_{MnO2}+\Phi_{DO}}\Phi_{MnO2} + K_{sedrel}SOD\frac{A}{V}$$

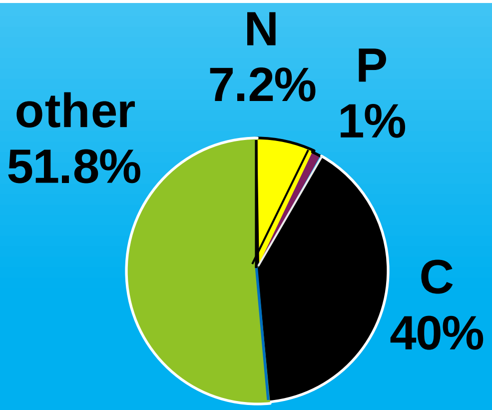
$$S_{FeII} = -K_{Fe}\Phi_{DO}\theta^{(PH-7)}\Phi_{FeII} + K_{FeOOH}\frac{K_{FeOOH}}{K_{FeOOH}+\Phi_{DO}}\Phi_{FeOOII} + K_{sedrel}SOD\frac{A}{V}$$

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

Water Quality: Organic Matter (OM) Constituents

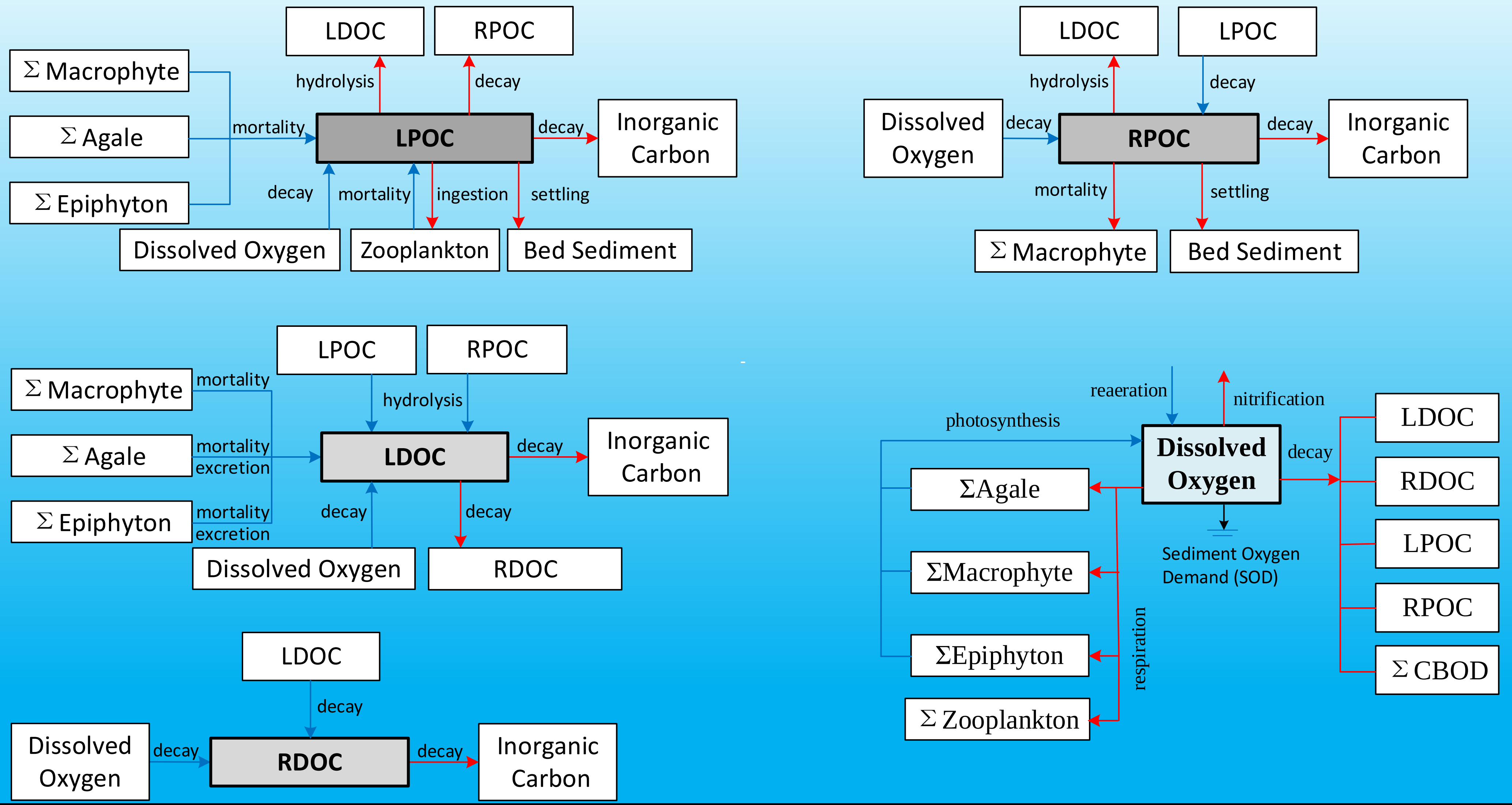






- Labile Particulate Organic Matter
- Refractory Particulate Organic Matter
- Labile Dissolved Organic Matter
- Refractory Dissolved Organic Matter

Water Quality: Organic Carbon (OC) Constituents

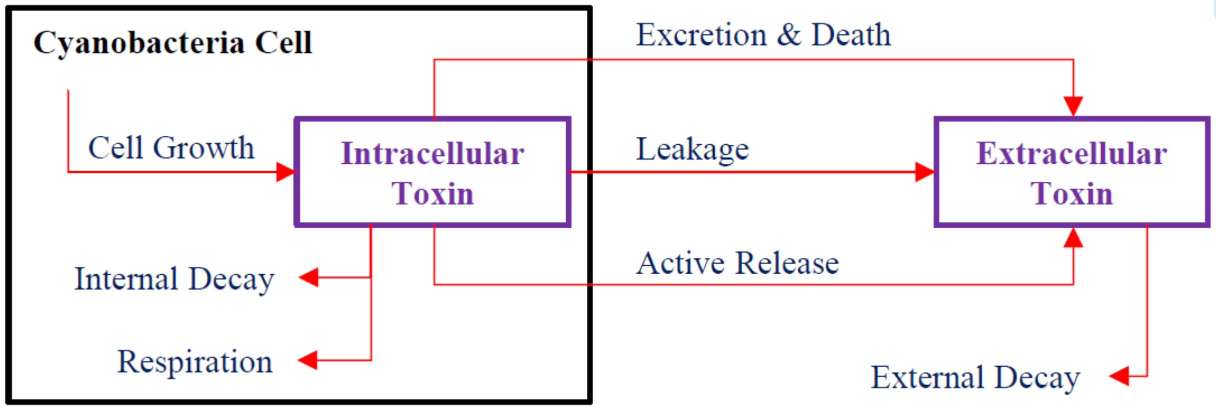


Water Quality: Algae Toxins

Four main toxins:

- Microcystin – hepatotoxin
- Cylindrospermopsin – cytotoxin
- Anatoxin-a – neurotoxin
- Saxitoxin – neurotoxin

1	Cyanotoxins Control File	ON/OFF	DEBUG	
2	TOXINCONTROL: ATOX (turn ON/OFF all algae toxins),ATOX_DEBUG (turn or	ON	ON	
3	MICROCYSTIN	ALG1	ALG2	ALG3
4	CTP_MC, fraction of algae concentration producing MC	0.5	0.25	0.3
5	CTB_MC, ratio of intracellular toxin to dry weight biomass (mg toxin/mg DW	0.1	0.2	0.2
6	CTR_MC, release rate, day-1	0.5		
7	CTD_MC, extracellular decay , day-1	0.1		
8	CYLINDROSPERMOPSIN	ALG1	ALG2	ALG3
9	CTP_CYN, fraction of algae concentration producing CYN	1	0	0
10	CTB_CYN, ratio of intracellular toxin to dry weight biomass (mg toxin/mg DV	0.25	0.2	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	ALG3
14	CTP_ATX, fraction of algae concentration producing ATX	0.5	0.25	0.3
15	CTB_ATX, ratio of intracellular toxin to dry weight biomass (mg toxin/mg DV	0.1	0.2	0.2
16	CTR_ATX, release rate, day-1	0.5		
17	CTD_ATX, extracellular decay, day-1	0.1		
18	SAXITOXIN	ALG1	ALG2	ALG3
19	CTP_STX, fraction of algae concentration producing STX	0.5	0.25	0.3
20	CTB_STX, ratio of intracellular toxin to dry weight biomass (mg toxin/mg DW	0.1	0.2	0.2
21	CTR_STX, release rate, day-1	0.5		
22	CTD_STX, extracellular decay , day-1	0.1		



$$C_{intra} = \sum_{i=1}^{n\ algal\ groups} a * \beta * (CTP)$$

$$\frac{dC_{extra}}{dt} = k_d * a * \beta * (CTP) + k_{release} * C_{intra} - k_{decay} * C_{extra}$$

CTP = fraction of algal group producing toxin

β = ratio of intra. toxin mass to mass of dry weight OM

Water Quality: Derived Variables

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

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

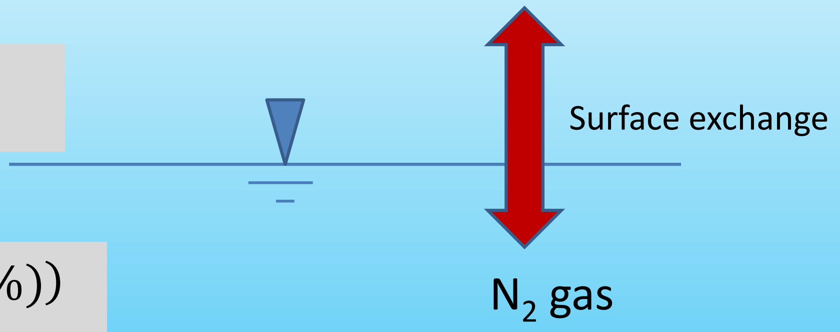
Secchi disk (m) is computed from λ (light extinction coefficient)

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

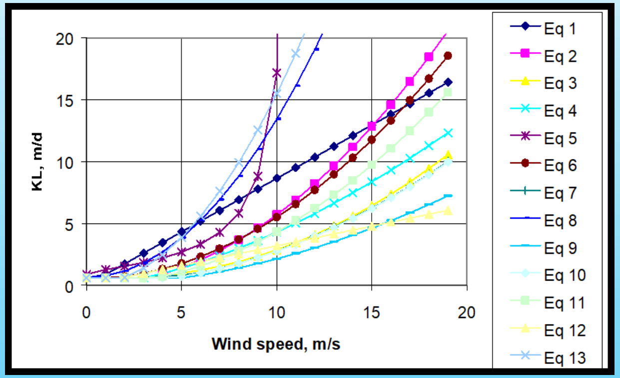
Total Dissolved Gas (TDG)

- Modeling N2 and DO

$$\frac{dN2}{dt} = -\frac{1}{h}k_{aN2}(N2 - N2_s)$$



$$TDG(\%) = (79N2(\%) - 21DO(\%))$$

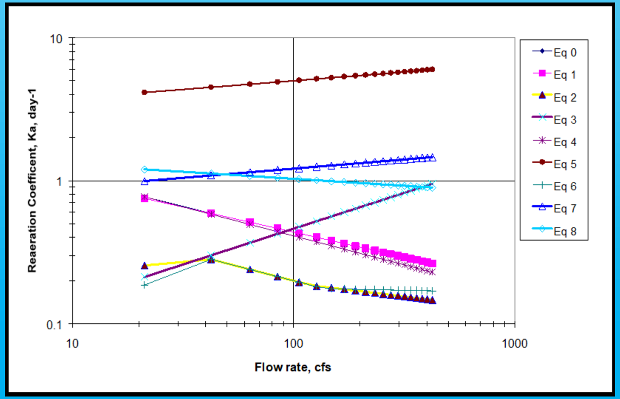


Lake/reservoir

- Modeling DGP (Dissolved Gas Pressure)

$$\frac{dDGP}{dt} = -k_{DGP}(DGP - PALT_{atm})$$

$$k_{DGP} = max(k_{DGP}, MINKL)$$



Stream/River

Amount of gas absorbed by water is proportional to its partial pressure in the atmosphere (conc. = solubility factor X partial pressure)

Total Dissolved Gas (TDG)/SYSTDG

- Dam Effects on Oxygen/Gas Transfer
  - Spillways, Weirs, and Gates
- SYSTDG is an Excel-based spreadsheet model used to compute TDG saturation levels in reservoir and riverine systems.

TDG production equations:

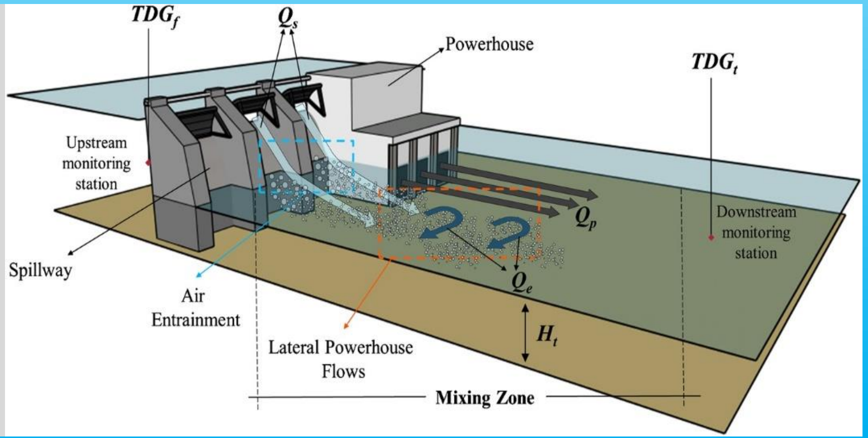
$$1.\ TDG_{sp} = 95.791 - 1.07193 * temp_{air} + 178.852 * (1 - e^{-0.51 * Q_{sp}}) + bp$$

$$2.\ TDG_{sp} = P1 * (twe - twce)^{P2} * \left(1 - e^{P3 * q_s}\right) + P4 + bp$$

$$3.\ TDG_{sp} = P1 * (twe - twce)^{P2} * {q_s}^{P3} + P4 + bp$$

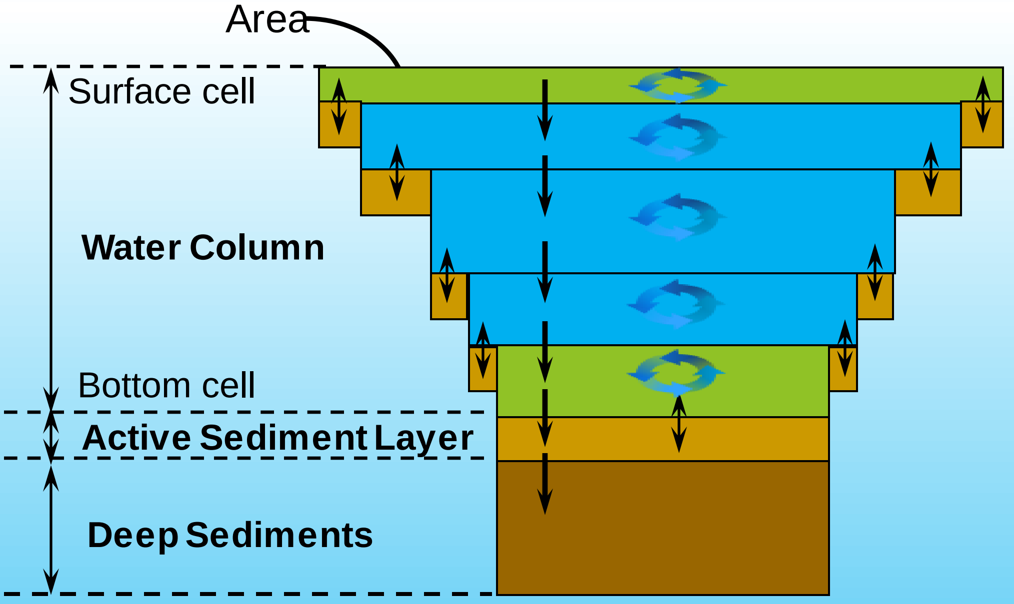
$$4.\ TDG_{sp} = P1 * (twe - twce) + P2 * {q_s}^{P3} + P4 + bp$$

$$5.\ TDG_{sp} = \mathrm{P1} * \left(1 - e^{\mathrm{P2} * q_s}\right) + \mathrm{P3} * (Temp_{tw} - P4) + \mathrm{bp}$$



$$TDG_{rel} = \frac{TDG_{sp}(Q_{sp}+Q_{ent})+TDG_{ph}(Q_{ph}-Q_{ent})}{Q_{ph}+Q_{sp}}$$

Sediment Compartment



Zero order sediment fluxes

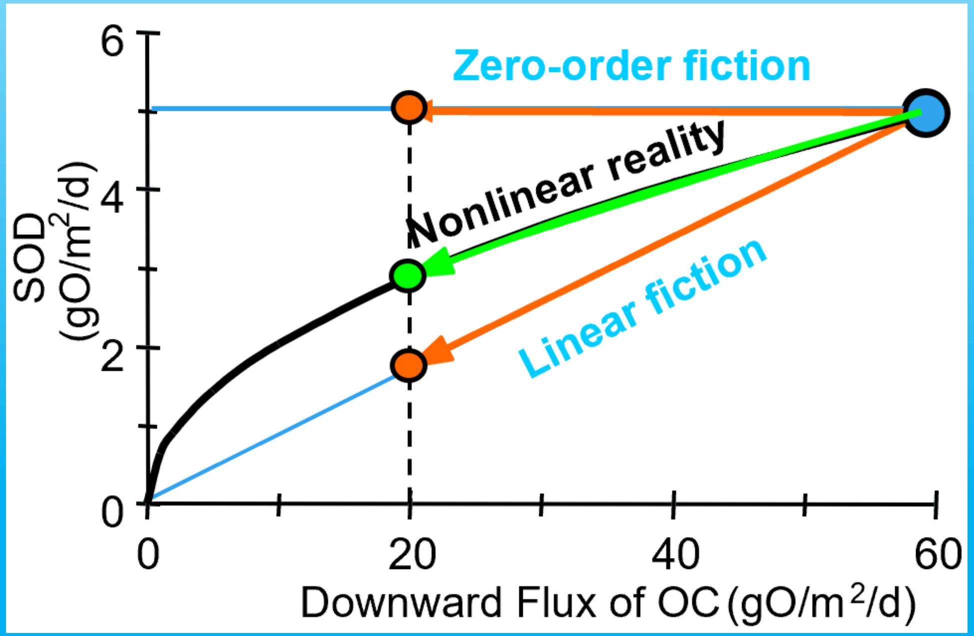
- Directly specify nutrient releases, with temperature adjustment
- Available in almost all water quality models

First order sediment fluxes

- Link fluxes to organic matter
- Limited application

Sediment diagenesis modeling

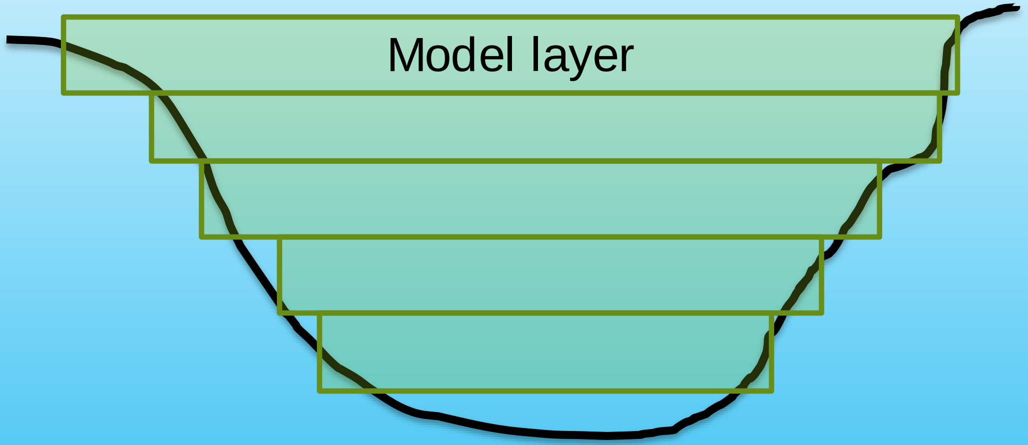
- Directly simulate the reactions in the sediment layer

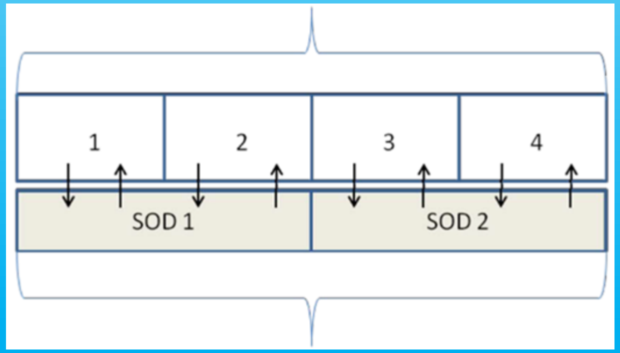


Courtesy of Steven Chapra

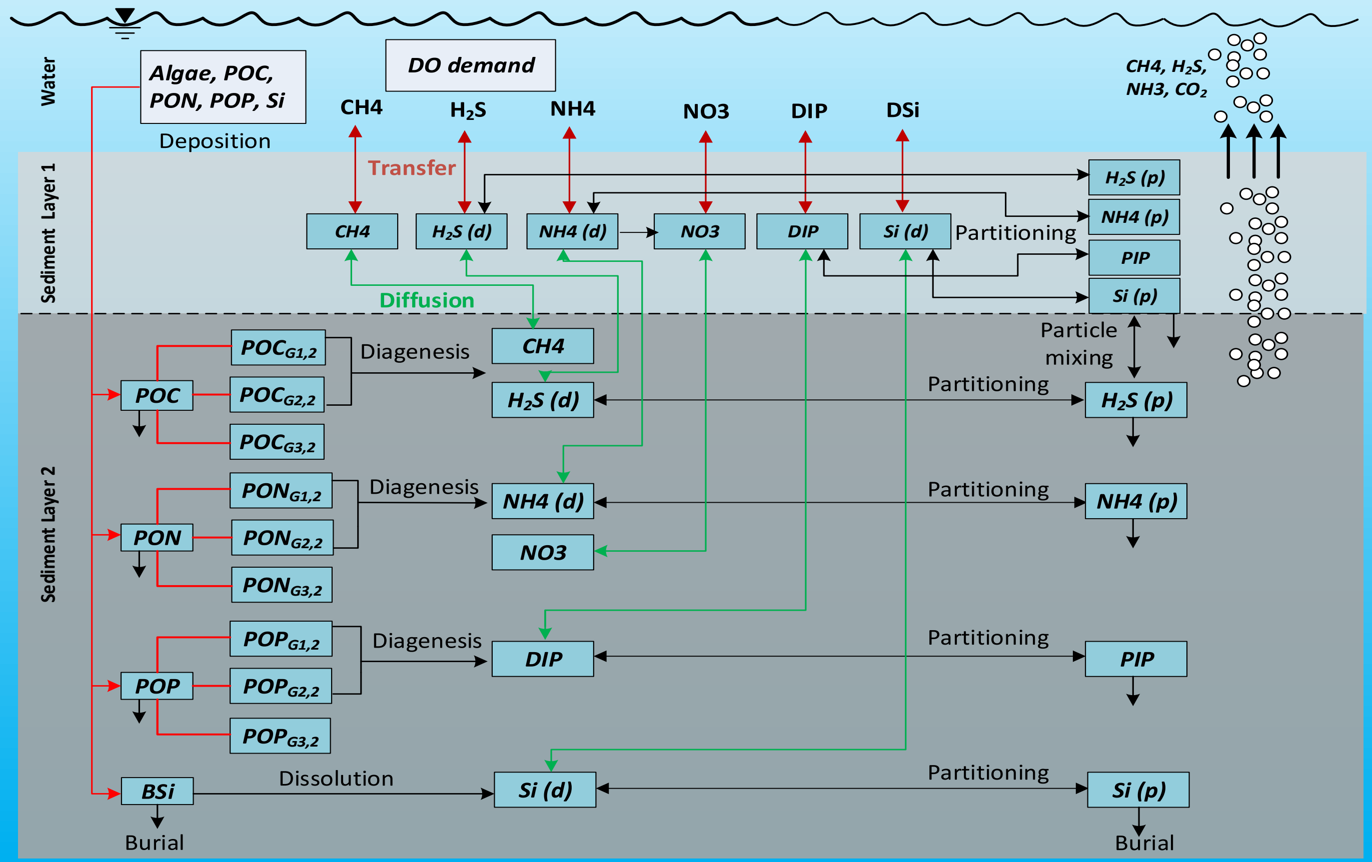
Sediment Diagenesis

- Inputs: csv format
- Outputs: Bottom layer and averaged outputs
- Improve the computations
- Add SOD and sediment fluxes for all water column layers
- Add initial conditions for NO3 in sediment layers
- Add sediment POM (POC, PON and POP) computation
- Add the correction for calculating SD_W12
- Add a correction for PO4 partitioning coefficient in layer 1
- Add partitioning of sediment NH4
- Modify the numerical solution for CH4





Sediment Diagenesis: State Variables and Processes



- 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

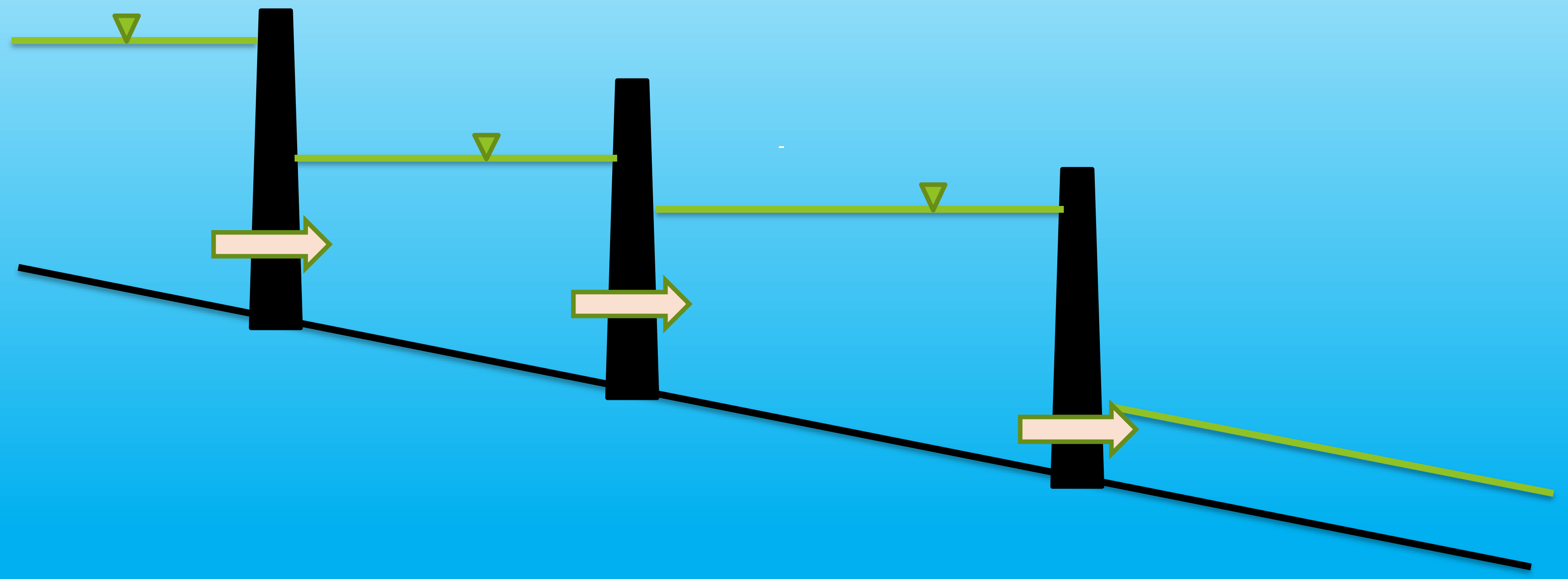
$ W2_diagenesis input file			
$ All lines at top of file starting with $ are comments and disregarded by the model			
$ Additional inputs are required if a group switch is ON			
$ Zhong Zhang, 7/21/21			
"Global Switch for all sediment diagenesis features"	.TRUE.		
"Include FFT layer (Fine Fluids Tailing - 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*

CE-QUAL-W2 Multi-Water Body Computation

Multiple waterbody simulation on multiple processors and preserving numerical precision improvements from 30-90%



CE-QUAL-W2 V4.5 Tools

1. **w2_con.xlsm** – develops W2 control files
2. **w2_v45_64.exe** – reads W2 inputs and execute the model
3. **preW2-v45_64.exe** – checks all W2 input files including the control file, bathymetry file, and all boundary condition files
4. **WaterBalanceConsole_45.exe** – performs the water balance calculation
5. **W2_Post.exe** – visualizes W2 model outputs
6. **ConverterControlFile.exe** – converts a previous version (V3.7 – V4.22) W2 control files into V4.5

Questions?