

# Updating the CEMA Oil Sands Pit Lake Model

**Prepared for:**

CEMA

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## Introduction

Cumulative Environmental Management Association (CEMA), a key advisor to the provincial and federal governments committed to making recommendations to manage the cumulative environmental effects of regional development on air, land, water and biodiversity, has undertaken to develop and enhance a water quality and hydrodynamic model for Oil Sands Pit Lakes.

The original development of the CEMA Oil Sands Pit Lake Model (OSPLM) was documented in ERM and Golder Associates (2011) and Prakash et al. (2011). This development incorporated a sediment diagenesis module, tailings consolidation, pore water release, biogenic gas production, bubble release, and salt rejection during ice formation within the CE-QUAL-W2 model Version 3.6 (Cole and Wells, 2008).

A peer review of the OSPLM revealed the need for coding updates and identified several new algorithms that would be useful to the model application (Wells, 2012). Hence, the Reclamation Water Group of CEMA decided to enhance the existing OSPLM. This model enhancement included updating the algorithms of the original CEMA OSPLM and adding new algorithms to the model. These updates included:

- Correcting code errors in the original OSPLM
- Updating the OSPLM to the current release version 3.71 and keep it in the recurring code base for future CE-QUAL-W2 updates
- Adding an algorithm for modeling phosphate in the sediments (this was not a part of the original OSPLM)
- Developing new algorithms for
  - modeling the sediment production of methane and sulfide within the water column
  - modeling the consumption of dissolved oxygen due to sediment re-suspension
  - modeling the dynamic calculation of sediment pH and temperature
  - modeling metal complexation and diagenesis

## Coding Updates to the OSPLM

Wells (2012) determined a list of coding issues or errors in the original OSPLM. Appendix A shows a list of coding issues that were corrected in this latest version of the OSPLM.

In addition to these issues, additional coding changes were made to improve and enhance the code. These additional coding additions are listed in Table 1 showing what routines were updated. Appendix B goes over changes in the input files and describes how to set up and run the new version of the OSPLM with the new algorithms. Descriptions of the new algorithms are shown in this report.

**Table 1 . Source code additions for OSPLM.**

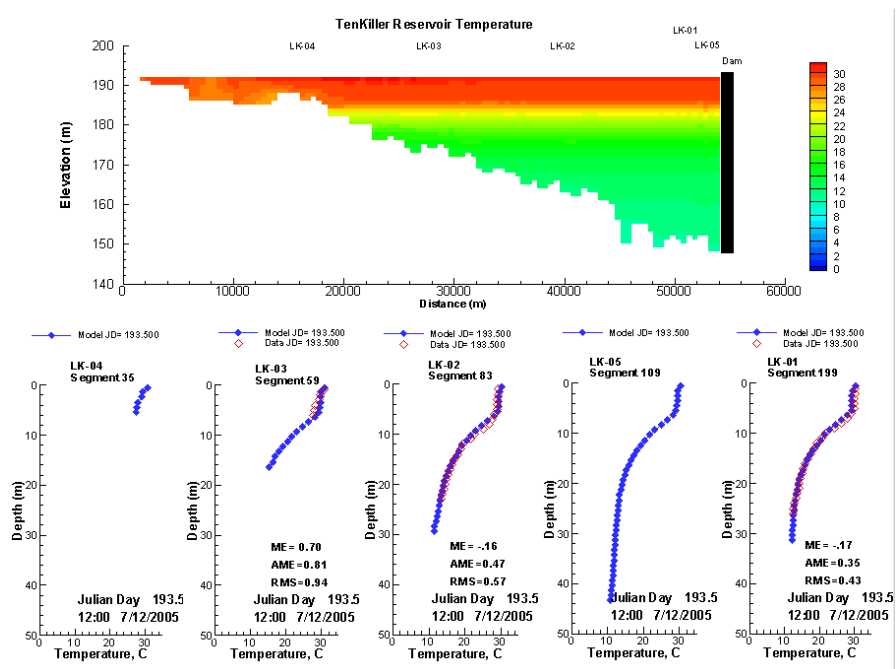
Code subroutine or entry point	Comment
CEMA_W2_Input	Expanded number of variables read from W2_CEMA.npt input files
INPUT	New variables for enhanced pH buffering and non-conservative alkalinity are read from pH_buffering.npt file
PH_CO2_NEW	Added enhanced pH buffering for water column
ALKALINITY	Added non-conservative alkalinity to sediments and water column
GENERIC_CONST	Modeling of hydrogen sulfide, methane, sulfate, manganese, manganese hydroxide, ferrous iron, and iron oxyhydroxide added for water column
DoCEMAMFTSedimentDiagen	Modeling of temperature, alkalinity, total inorganic carbon, phosphorus, manganese, manganese hydroxide, ferrous iron, and iron oxyhydroxide added for sediments
W2modules_par.f90	Expanded number of variables in module CEMAVars
CEMASedimentDiagenesis	Added variables for modeling of new constituents. Variables are also initialized.
CEMAMFTSedimentFluxModel	Added variables for modeling of new constituents.
UpdateCEMASedimentFluxVariables	Added variables for modeling of new constituents.
WriteCEMASedimentFluxVariables	Added variables for modeling of new constituents.
PH_SEDIMENTS	Added enhanced pH buffering in sediments
WQCONSTITUENTS	Inserted new calls for enhanced pH buffering and non-conservative alkalinity

## CE-QUAL-W2 Version Update

The base CE-QUAL-W2 model used for the OSPLM was updated from Version 3.6 to Version 3.7. The original Version 3.6 OSPLM was developed by ERM and Golder Associates (2011). There have been many model enhancements between Version 3.6 and Version 3.71 (Cole and Wells, 2013).

### CE-QUAL-W2 Background

CE-QUAL-W2 version 3.71 (Cole and Wells, 2013) is a public domain model. It is a 2-dimensional (longitudinal-vertical) hydrodynamic and water quality model capable of predicting water surface elevation, velocity, temperature, nutrient concentrations, multiple algae, zooplankton, periphyton, and macrophyte species, dissolved oxygen, pH, alkalinity, multiple CBOD groups, multiple suspended solids groups, multiple generic constituents (such as tracer, bacteria, toxics), and multiple organic matter groups, both dissolved and particulate. The model is set up to predict these state variables at longitudinal segments and vertical layers (see Figure 1).



**Figure 1** CE-QUAL-W2 model predictions for Tenkiller Reservoir, OK, USA, for temperature as a function of depth and longitudinal distance on July 12, 2005. Field data are red symbols compared to the blue model profile predictions.

Typical model longitudinal resolution is between 100-1000 m; vertical resolution is usually between 0.5 m and 2 m. The model can also be used in quasi-3-D mode, where embayments are treated as separate model branches off the main stem of the reservoir. The user manual and documentation can be found at the PSU website for the model: <http://www.cee.pdx.edu/w2>.

Dr. Wells and his group have been the primary developers of this model for the ERDC (Engineer Research and Development Center), Environmental Laboratory, Waterways Experiments Station Corps of Engineers for the last 15 years. Since 2000, this model has been used extensively throughout the world in a wide range of applications (see Table 1).

**Table 2. CE-QUAL-W2 applications between 2000-2006.**

<b>Water body</b>	<b>Approximate Number of Applications</b>
Reservoirs	500
Lakes	400
Rivers	500
Estuaries	100
Pit Lakes	20

Between June 2004 and June 2012 there have been about 8500 model downloads or about 1000/year from 159 countries. Of these downloads, 4020 were for Version 3.6, the prior model version. Most downloads were from (in order): USA, Iran, Korea, China, Brazil, Canada, Germany, India, Australia, Portugal, and Columbia. Version 3.7 was released at the end of 2012 that included a new post-processor from DSI.

## **Model Changes between Version 3.6 and Version 3.7.1**

### **Version 3.7**

Many of the code revisions for Version 3.7 were made to extend the usefulness of the model in analysis of complex water quality and temperature applications.

1. The model has been improved to handle river flow regimes. These model enhancements for river systems include the following:
  - a. The initial water surface elevation of a river system based on the normal depth of the river is computed within the model. This allows the model to run more smoothly from the start and eliminates trying to guess an initial water surface elevation for a river system.
  - b. The model in earlier versions assumed that the initial velocity regime was 'zero'. By computing an initial velocity regime based on the initial conditions of the flows, the river model then starts with a non-zero velocity. This allows the model to run more smoothly from the very beginning of the model simulation.
  - c. The model user can choose 'Trapezoidal' or 'Rectangular' model segments. This will allow for a smoother transition as water levels move up and down in a river channel. This should also allow for a larger maximum time step for stability in the river system.
  - d. The model user can now specify 2 slopes for a model branch. One slope is the slope of the elevation grid for which all elevations are tied together. The other slope is the hydraulic equivalent slope of a channel. In other words, if a model branch includes riffles and pools, the actual grid slope may not be the equivalent hydraulic slope.
2. There is a new bathymetry file input format that is easily developed using 'Excel'. This simplifies setting up the initial grid and debugging it.



3. Temperature and dissolved oxygen habitat volumes are now computed within the model for different fish species.
4. There is a new selective withdrawal algorithm that will select the elevation of the withdrawal necessary to meet temperature targets.
5. Since each BOD group can have a different BOD-P, BOD-C and BOD-N stoichiometric equivalent, it was necessary to add to the model new state variables, BOD-P, BOD-N, and BOD-C that allowed for time variable inputs of BOD-P, BOD-C and BOD-N from a point or non-point source.
6. Environmental performance criteria were developed to evaluate time and volume averages over the system of state variables chosen for analysis. This is an easy method for looking at water quality differences between model runs.
7. The model now has a module for adding dissolved oxygen, such as hypolimnetic aeration, to specific locations based on a dynamic dissolved oxygen probe monitoring the dissolved oxygen levels.
8. The model also has a dynamic pipe algorithm allowing a pipe to be turned ON or OFF over time, as if a gate was closed.
9. The model also has a dynamic pump algorithm that allows the model user to set dynamic parameters for the water level control over time. This is very useful in setting rule curves for operation of the reservoir water levels over time.
10. The maximum time step can now be set to interpolate its value over time rather than suddenly changing the maximum time step. This allows for a smoother change in the model time step.
11. The computation of the temperature at which ice freezes has been adjusted to account for salt water impacts. [Courtesy of Dr. Ray Walton]
12. New model output includes volume weighted averages of eutrophication water quality variables as a function of segment and for only surface conditions as specified by the model user. Other new output includes output of flows, concentrations, and temperatures from a segment for all individual withdrawals.

## Version 3.71

This version is file compatible with version 3.7 but does add one new variable to the control file w2\_con.npt.

1. New model input formats (free format) for many input files that were in fixed format. The new files allow for much easier model file development in Excel. These new files include the following files:

- a. All concentration input files for inflows, tributaries, distributed tributaries and precipitation:
  - i. Cin files
  - ii. Ctrib files
  - iii. Cdtrib files
  - iv. Cpre files
- b. Wind sheltering file
  - i. Wsc file
- c. Meteorological input file
  - i. Met file
- d. Vertical profile file for initial condition
  - i. Vpr file
- e. Longitudinal-vertical profile initial condition
  - i. Lpr file
- f. Withdrawal flow file
  - i. Qwd file
- g. Structure outflow file
  - i. Qot file
- h. Flow and temperature input files for
  - i. Qin and Tin
  - ii. Qtrib and Ttrib
  - iii. Qdtrib and Tdtrib

2. New option for dynamic outlet structure elevation for each model structure. Hence, the centerline elevation of the structure can be variable over time. In the control file, there is an ON/OFF option after declaring the # of structures for each branch.
3. The release of a new post-processor from DSI, Inc. that uses the vector output in w2\_con.npt to specify frequency of output for this post-processor.

By updating the model to the current release version of the CE-QUAL-W2 model, the code itself will be maintained in the release version so that all model updates will be available to users of the CE-QUAL-W2 model.

## Sediment Phosphorus

As coding changes were made to the original OSPLM, it became clear that P (Phosphorus) release from the sediments was not completed or implemented in the model. In order to have a complete model, P release mechanisms were developed for the OSPLM. A schematic of the sediment phosphate model is shown in

Figure 2. Figure 3 and Figure 4 show the phosphate sources and sinks in the aerobic and anaerobic compartments, respectively, in the CE-QUAL-W2 model framework.

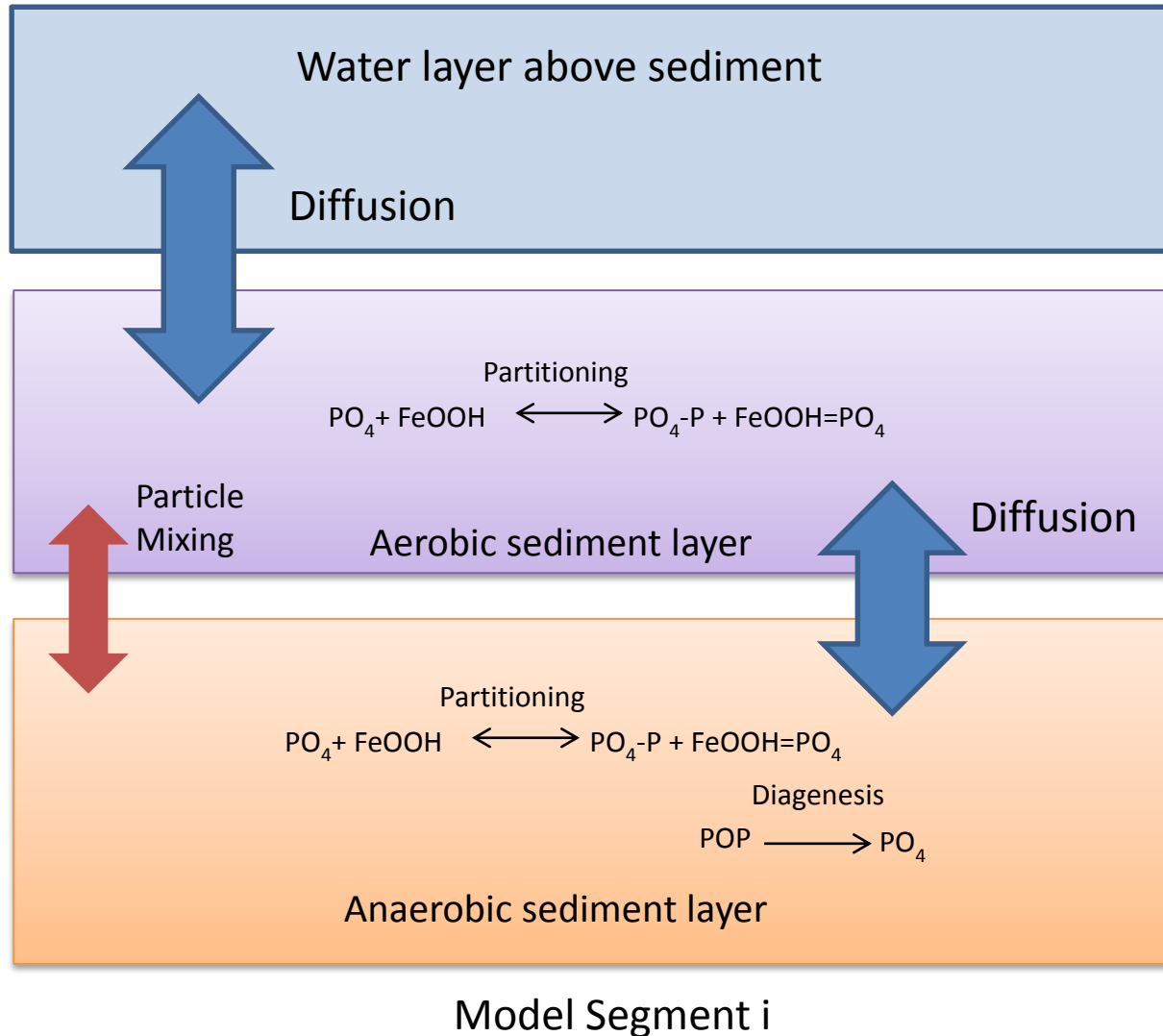
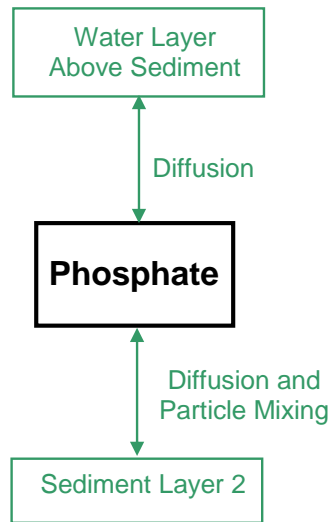
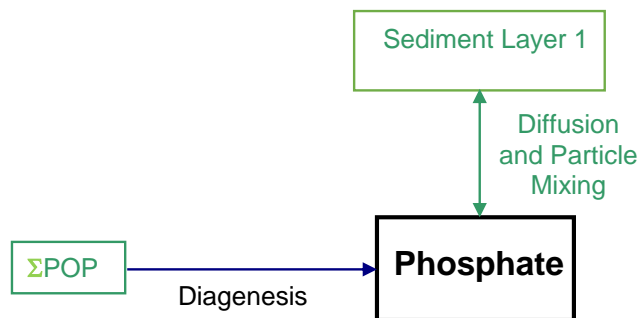


Figure 2. Schematic of sediment phosphate model (Ditoro, 2001).



**Figure 3 Internal flux between phosphate within the aerobic sediment layer 1 and other compartments**



**Figure 4 Internal flux between phosphate within the anaerobic sediment layer 2 and other compartments**

Because the aerobic layer is assumed to be very thin, oxidation of particulate organic phosphorus is assumed to be negligible. The source/sink rate equation for phosphate in sediment layer 1 is assumed to be zero:

$$S_{PO41} = 0$$

The rate equation for phosphate in sediment layer 2 is:

$$S_{PO42} = \underbrace{\sum_{i=1}^3 k_{POPi} \gamma_{POP} \Phi_{POPi}}_{\text{Diagenesis}}$$

where

$\gamma_{POP}$  = particulate organic phosphorus temperature rate multiplier

$k_{POPi}$  = particulate organic phosphorus class  $i$  mineralization rate,  $\text{sec}^{-1}$

$\Phi_{POPi}$  = particulate organic carbon class  $i$  concentration,  $g\ m^{-3}$

The three classes correspond to labile, refractory, and inert/slow refractory particulate organic phosphorus for  $i=1$ ,  $i=2$ , and  $i=3$ , respectively. Phosphate can exist in dissolved and particulate forms. Dissolved oxygen concentrations determine the extent to which dissolved phosphate sorbs to iron oxyhydroxide particulates. Within the aerobic layer phosphate sorbs to iron oxyhydroxide. At low dissolved oxygen concentrations, iron oxyhydroxide is reduced and the sorbed phosphate is released.

Mass balance equations for layer 1 (aerobic) and layer 2 (anaerobic) are:

$$H_1 \frac{d\Phi_{PO41}}{dt} = -K_{L01}(f_d \Phi_{PO41} - \Phi_{PO40}) + K_{L12}(f_d \Phi_{PO42} - f_d \Phi_{PO41}) + w_{12}(f_p \Phi_{PO42} - f_p \Phi_{PO41}) - w_2 \Phi_{PO41}$$

$$H_2 \frac{d\Phi_{PO42}}{dt} = -K_{L12}(\Phi_{PO42} - \Phi_{PO41}) - w_{12}(f_p \Phi_{PO42} - f_p \Phi_{PO41}) + w_2(\Phi_{PO41} - \Phi_{PO42}) + H_2 S_{PO42}$$

where

$\Phi_{PO41}$  = total phosphate concentration in layer 1,  $g\ m^{-3}$

$\Phi_{PO42}$  = total phosphate concentration in layer 2,  $g\ m^{-3}$

$\Phi_{PO40}$  = phosphate concentration in water column,  $g\ m^{-3}$

$H_1$  = height of layer 1,  $m$

$H_2$  = height of layer 2,  $m$

$K_{L01}$  = mass transfer coefficient between water column and layer 1,  $m\ s^{-1}$

$K_{L12}$  = mass transfer coefficient between layer 1 and layer 2,  $m\ s^{-1}$

$f_d$  = dissolved fraction of phosphate

$f_p$  = particulate fraction of phosphate

$w_{12}$  = particle mixing velocity between layer 1 and layer 2,  $m\ s^{-1}$

$w_2$  = burial velocity,  $m\ s^{-1}$

The implicit finite difference scheme for layer 1 is

$$H_1 \frac{\Phi_{PO41}^{t+\Delta t} - \Phi_{PO41}^t}{\Delta t} = -K_{L01}(f_d \Phi_{PO41}^{t+\Delta t} - \Phi_{PO40}) + K_{L12}(f_d \Phi_{PO42}^{t+\Delta t} - f_d \Phi_{PO41}^{t+\Delta t}) + w_{12}(f_p \Phi_{PO42}^{t+\Delta t} - f_p \Phi_{PO41}^{t+\Delta t}) - w_2 \Phi_{PO41}^{t+\Delta t}$$

Rearranging

$$\begin{aligned} & \left( -\frac{H_1}{\Delta t} - f_d K_{L01} - f_d K_{L12} - w_{12} f_p - w_2 \right) \Phi_{PO41}^{t+\Delta t} + (K_{L12} f_d + w_{12} f_p) \Phi_{PO42}^{t+\Delta t} \\ & = -\frac{H_1}{\Delta t} \Phi_{PO41}^t - K_{L01} \Phi_{PO40} \end{aligned}$$

And the finite difference scheme for layer 2

$$\begin{aligned} H_2 \frac{\Phi_{PO42}^{t+\Delta t} - \Phi_{PO42}^t}{\Delta t} & = -K_{L12} (f_d \Phi_{PO42}^{t+\Delta t} - f_d \Phi_{PO41}^{t+\Delta t}) - w_{12} (f_p \Phi_{PO42}^{t+\Delta t} - f_p \Phi_{PO41}^{t+\Delta t}) \\ & + w_2 (\Phi_{PO41}^{t+\Delta t} - \Phi_{PO42}^{t+\Delta t}) + H_2 S_{PO42} \end{aligned}$$

Rearranging

$$(f_d K_{L12} + f_p w_{12} + w_2) \Phi_{PO41}^{t+\Delta t} + \left( -\frac{H_2}{\Delta t} - f_d K_{L12} - f_p w_{12} - w_2 \right) \Phi_{PO42}^{t+\Delta t} = -H_2 S_{PO42} - \frac{H_2}{\Delta t} \Phi_{PO42}^t$$

The fractions associated with dissolved and particulate forms can be calculated with (Chapra, 1997):

$$\begin{aligned} f_d & = \left( \frac{1}{\varphi + K_{dp}(1 - \varphi)\rho} \right) \\ f_p & = \left( \frac{K_{dp}(1 - \varphi)\rho}{\varphi + K_{dp}(1 - \varphi)\rho} \right) \end{aligned}$$

Where

$f_d$  = dissolved fraction of phosphate

$f_p$  = particulate fraction of phosphate

$\varphi$  = sediment porosity

$\rho$  = sediment density,  $g\ m^{-3}$

$K_{dp}$  = phosphorus sorption coefficient,  $m^3\ g^{-1}$

## Sediment Production of Methane and Sulfide

The modeling of methane (CH<sub>4</sub>) and hydrogen sulfide (H<sub>2</sub>S) constituents were added to the water column. CH<sub>4</sub> is modeled as mg/l as C. H<sub>2</sub>S is modeled as mg/l as S. For both constituents, the anaerobic release from the sediments, aerobic decay, and reaeration were modeled (Figure 5).

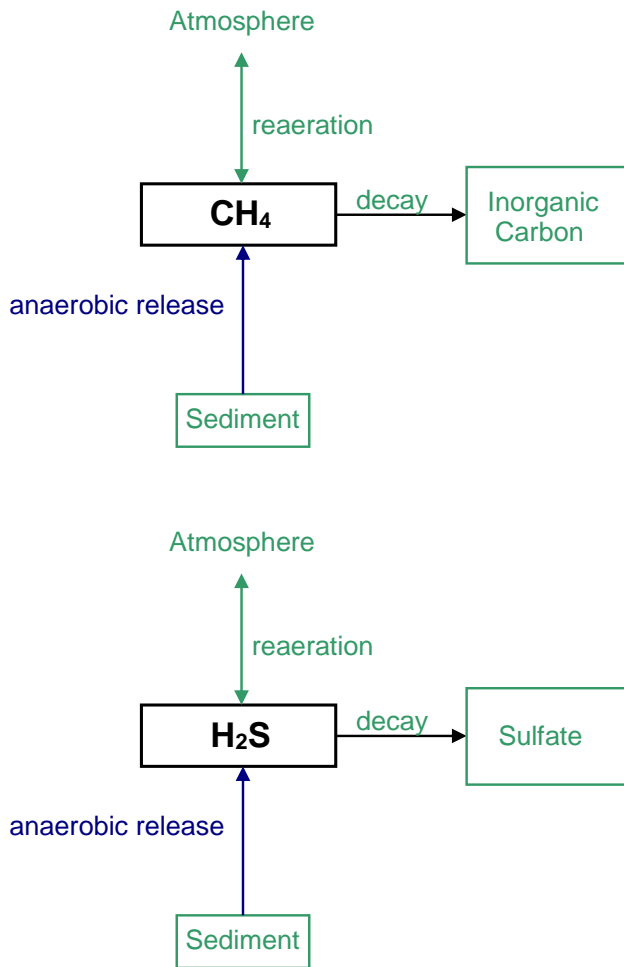


Figure 5. Sources and sinks for methane and hydrogen sulfide.

The rate equations for methane and hydrogen sulfide were identical (assuming saturation values in the atmosphere of 0 mg/l for both gases):

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

where:

$A_{sed}$  = sediment surface area,  $m^2$

$A_{sur}$  = surface area of surface computational cell,  $m^2$   
 $SOD$  = sediment oxygen demand,  $g\ m^{-2}\ sec^{-1}$   
 $K_L$  = interfacial exchange rate,  $m\ sec^{-1}$   
 $\gamma_{OM}$  = organic matter temperature rate multiplier  
 $\delta_{SODR}$  = sediment release rate of  $H_2S$  or  $CH_4$ , fraction of SOD  
 $\Phi$  = constituent concentration ( $H_2S$  or  $CH_4$ ),  $g\ m^{-3}$   
 $\Theta$  = temperature rate multiplier  
 $T$  = temperature,  $^{\circ}C$   
 $K$  = decay rate,  $sec^{-1}$

The basic physics of gas transfer are the same for  $H_2S$ ,  $CH_4$  and  $O_2$ . Using the penetration theory for gas transfer, i.e.,  $K_a = 2\sqrt{\frac{Df}{\pi}} \frac{1}{h}$  where  $f$  is the turbulence frequency of surface renewal,  $D$  is the molecular diffusion coefficient for  $O_2$  and  $h$  is the depth, once the reaeration coefficient for dissolved oxygen is determined, then the value of the reaeration coefficient  $k_{H_2S}$  for  $H_2S$  is determined from the following equation (Thibodeaux, 1996):

$$k_{H_2S} = k_{O_2} \sqrt{\frac{D_{H_2S}}{D_{O_2}}}$$

Using

$$\frac{D_A}{D_B} = \sqrt{\frac{MW_B}{MW_A}} \text{ where MW is the molecular weight of the component}$$

then

$$k_{H_2S} = k_{O_2} \left( \frac{MW_{O_2}}{MW_{H_2S}} \right)^{0.25}.$$

Given the molecular weights of oxygen and hydrogen sulfide :

$$MW_{O_2} = 32.00\ g/mol$$

$$MW_{H_2S} = 34.08\ g/mol$$

the reaeration coefficient for hydrogen sulfide is:

$$k_{H_2S} = k_{O_2} \left( \frac{MW_{O_2}}{MW_{H_2S}} \right)^{0.25} = k_{O_2} \times 0.984$$



Likewise for methane

$$MW_{CH_4} = 16.04 \text{ g/mol}$$

The reaeration coefficient  $k_{CH_4}$  is:

$$k_{CH_4} = k_{O_2} \left( \frac{MW_{O_2}}{MW_{CH_4}} \right)^{0.25} = k_{O_2} \times 1.188$$

## Consumption of Dissolved Oxygen due to Sediment Resuspension

Particulate organic matter in the sediments can be resuspended by turbulence caused by wind or by bottom scour caused by high current velocities. Once particulate organic matter has been re-suspended into an aerobic water column, it will decay and consume dissolved oxygen.

### Wind Induced Resuspension

This algorithm for predicting the resuspension of particulate organic matter due to wind is based on work from Kang et al. (1982) where the bottom shear stress is computed based on wind speed, wind fetch and depth. The wind blowing across a water surface creates wind waves that have orbital motion that decays with depth. The model user inputs a critical shear stress for detachment of the particles. If the critical shear stress is exceeded, then particles are resuspended. The approach of Kang et al. (1982) consists of the following steps:

1. Computation of the wave height,  $H_s$  in m,

$$H_s = \frac{W^2}{g} 0.283 \tanh \left[ 0.53 \left( \frac{gH}{W^2} \right)^{0.75} \right] \tanh \left[ \frac{0.0125 \left( \frac{gF}{W^2} \right)^{0.42}}{\tanh \left[ 0.53 \left( \frac{gH}{W^2} \right)^{0.75} \right]} \right]$$

where  $W$  is the wind velocity (m/s),  $F$  is the fetch (m),  $H$  is the mean depth (m)

2. Computation of wave period,  $T_s$  in s,

$$T_s = \frac{2\pi W}{g} 1.2 \tanh \left[ 0.833 \left( \frac{gH}{W^2} \right)^{0.375} \right] \tanh \left[ \frac{0.077 \left( \frac{gF}{W^2} \right)^{0.25}}{\tanh \left[ 0.833 \left( \frac{gH}{W^2} \right)^{0.375} \right]} \right]$$

Computation of the wavelength,  $L$  in m, iteratively from the following equation:

$$L = \frac{gT_s^2}{2\pi} \tanh \left[ \frac{2\pi H}{L} \right]$$

Computation of the orbital velocity,  $\bar{U}$  in cm/s,

$$\bar{U} = \frac{\pi H_s}{T_s} \frac{100}{\sinh(2\pi H / L)}$$

Computation of bottom shear stress,  $\tau$  in dynes/cm<sup>2</sup>,

$$\tau = 0.003\overline{U}^2$$

Computation of actual bottom scour rate of suspended solids,  $\varepsilon$  in mass of sediments scoured per area or g/m<sup>2</sup>,

$$\varepsilon = 0 \quad \tau \leq \tau_c$$

$$\varepsilon = \frac{\alpha_o}{t_d^2} (\tau - \tau_c)^3 \quad \tau > \tau_c$$

where  $\alpha_o$  is an empirical constant=0.008,  $t_d=7$ , and  $\tau_c$  is the user-defined critical shear stress. Resuspension supposedly only occurs during the first hour of the wind shear greater than the critical shear

stress. Hence, the rate of resuspension per time,  $E$  in g/m<sup>2</sup>/hour, would be  $E = \frac{\varepsilon}{1hr}$  for the first hour and

nothing after that. The resulting concentration of suspended solids in the entire water column,  $c$  in mg/l, if distributed evenly over the entire volume would then be

$$c = \frac{10000\varepsilon A_{bottom}}{V} = \frac{10000\varepsilon}{H}.$$

where  $A_{bottom}$  is the surface area of the bottom and  $V$  is the volume of the water column above the bottom ( $=HA_{bottom}$ ). Chapra (1997) also uses this approach.

## Bottom Scour Resuspension

Following the approach of Edinger (2002) in the 3D model GLLVHT, the CE-QUAL-W2 model can compute the bottom scour of sediment (inorganic or organic) in units of g/m<sup>2</sup>/s from Nielson (1992) as

$$\text{Bottom scour rate} \left[ \frac{M}{L^2T} \right] = V_{scour} C_{bottom}$$

where the scour velocity  $V_{scour}$  (m/s) is calculated from

$$V_{scour} = \frac{0.00033 \left( \frac{\theta'}{\theta_c} - 1 \right) (S_g - 1)^{0.6} g^{0.6} d^{0.8}}{\nu}$$

and

$g$ = acceleration due to gravity, 9.78 m<sup>2</sup>/s

$d$ = particle diameter, m

$\theta'$ = Shield's parameter,  $\theta' = \frac{\tau_{bottom}}{[g(S_g-1)d]}$

$\theta_c$ =critical Shield's parameter [User input for each particle size]

$\tau_{bottom}$ = bottom shear stress in m<sup>2</sup>/s<sup>2</sup>, when using the Chezy coefficient,  $\tau_{bottom} = \frac{gU_{bottom}^2}{C^2}$

$U_{bottom}$ = bottom velocity, m/s

$C$ = Chezy coefficient in units, m<sup>0.5</sup>/s

$S_g$ = specific gravity of solid,  $\rho_{solid}/\rho_{water}$

$\nu$ = molecular viscosity of water,  $\nu = 1.79E - 6 \exp(-0.0266T)$

$C_{bottom}$  = bottom sediment concentration in mg/l,  $C_{bottom} = C_{KB} \exp\left(\frac{V_s \Delta z}{D_z}\right)$  or a minimum bottom concentration defined between 1.0 mg/l (0.02 mm particle diameter and  $S_g=1.2$ ), 3.0 mg/l (0.2 mm particle diameter and  $S_g=1.8$ ), and 5.0 mg/l (2.0 mm particle diameter and  $S_g=2.2$ ) [from Schubel et al. (1978)]

$V_s$  = settling velocity of particles, m/s

$\Delta z$  = vertical grid spacing at the bottom, m

$C_{KB}$  = Bottom concentration of suspended solids, mg/l

$D_z$  = vertical mass turbulent diffusion coefficient,  $m^2/s$

$T$  = water temperature, °C

The model user can input a value of critical Shields parameter in the control file or one can have the model estimate it based on the following approach. Cao et al. (2006) used a simple estimate of the critical Shield's parameter based on the particle Reynolds number explicitly. The particle Reynolds number,  $R$ , is defined as

$$R = d \sqrt{S_g g d}$$

The critical Shield's criterion is then

$$\theta_c = \frac{[1 + (0.0223R)^{2.8358}]^{0.3542}}{3.0946R^{0.6769}} \text{ for } R \text{ between } 6.6 \text{ and } 282.8$$

$$\theta_c = 0.1414R^{-0.2306} \text{ for } R < 6.6$$

$$\theta_c = 0.045 \text{ for } R > 282.8$$

## Mass Balance Equations for Particulate Organic Matter

The loss of particulate organic matter to the water column due to resuspension needs to be included in the mass balance equations for particulate organic carbon (POC), particulate organic nitrogen (PON), and particulate organic phosphorus (POP). The mass balance equation for POC in the anaerobic layer (layer 2) is (DiToro, 2001):

$$H_2 \frac{d\Phi_{POCi}}{dt} = -k_{POCi} \theta_{POCi}^{(T-20)} \Phi_{POCi} H_2 - w_2 \Phi_{POCi} + f_{POCi} J_{POC} - E_{POCi}$$

where

$\Phi_{POCi}$  = POC concentration in reactivity class  $i$  in layer 2,  $g\ m^{-3}$

$H_2$  = height of layer 2,  $m$

$J_{POC}$  = depositional flux of POC from water column,  $g\ m^{-2}\ s^{-1}$

$E_{POCi}$  = resuspension rate of reactivity class  $i$ ,  $g\ m^{-2}\ s^{-1}$

$k_{POCi}$  = reaction rate of reactivity class  $i$ ,  $s^{-1}$

$f_{POCi}$  = fraction of  $J_{POC}$  that is in reactivity class  $i$

$\theta_{POCi}$  = temperature coefficient for reactivity class  $i$

$T_2$  = temperature of layer 2, °C

$w_2$  = burial velocity,  $m\ s^{-1}$

And the finite difference scheme for layer 2

$$H_2 \frac{\Phi_{POCi}^{t+\Delta t} - \Phi_{POCi}^t}{\Delta t} = -k_{POCi} \theta_{POCi}^{(T-20)} \Phi_{POCi}^{t+\Delta t} H_2 - w_2 \Phi_{POCi}^{t+\Delta t} + f_{POCi} J_{POC} - E_{POCi}$$

Rearranging

$$H_2 \frac{\Phi_{POCi}^{t+\Delta t}}{\Delta t} + k_{POCi} \theta_{POCi}^{(T-20)} \Phi_{POCi}^{t+\Delta t} H_2 + w_2 \Phi_{POCi}^{t+\Delta t} = H_2 \frac{\Phi_{POCi}^t}{\Delta t} + f_{POCi} J_{POC} - E_{POCi}$$

And solving for  $\Phi_{POCi}^{t+\Delta t}$ :

$$\Phi_{POCi}^{t+\Delta t} = \left( \Phi_{POCi}^t + \frac{\Delta t}{H_2} f_{POCi} J_{POC} - \frac{\Delta t}{H_2} E_{POCi} \right) \left( 1 + \frac{w_2 \Delta t}{H_2} + k_{POCi} \theta_{POCi}^{(T-20)} \Delta t \right)^{-1}$$

The mass balance equations for PON and POP would be solved for in analogous fashion.

## Dynamic Calculation of Sediment pH and Temperature

### pH

The dynamic calculation of pH in the OSPLM was implemented using a similar approach as a pH model developed by the United States Geological Survey (Sullivan et al, 2013). In order to calculate pH, sediment organic carbon, sediment alkalinity, and sediment temperature also had to be modeled.

### Sediment Total Inorganic Carbon

A schematic of the sediment total inorganic carbon model is shown in Figure 6. Figure 7 and Figure 8 show the total inorganic carbon sources and sinks in the aerobic and anaerobic compartments, respectively, in the CE-QUAL-W2 model framework.

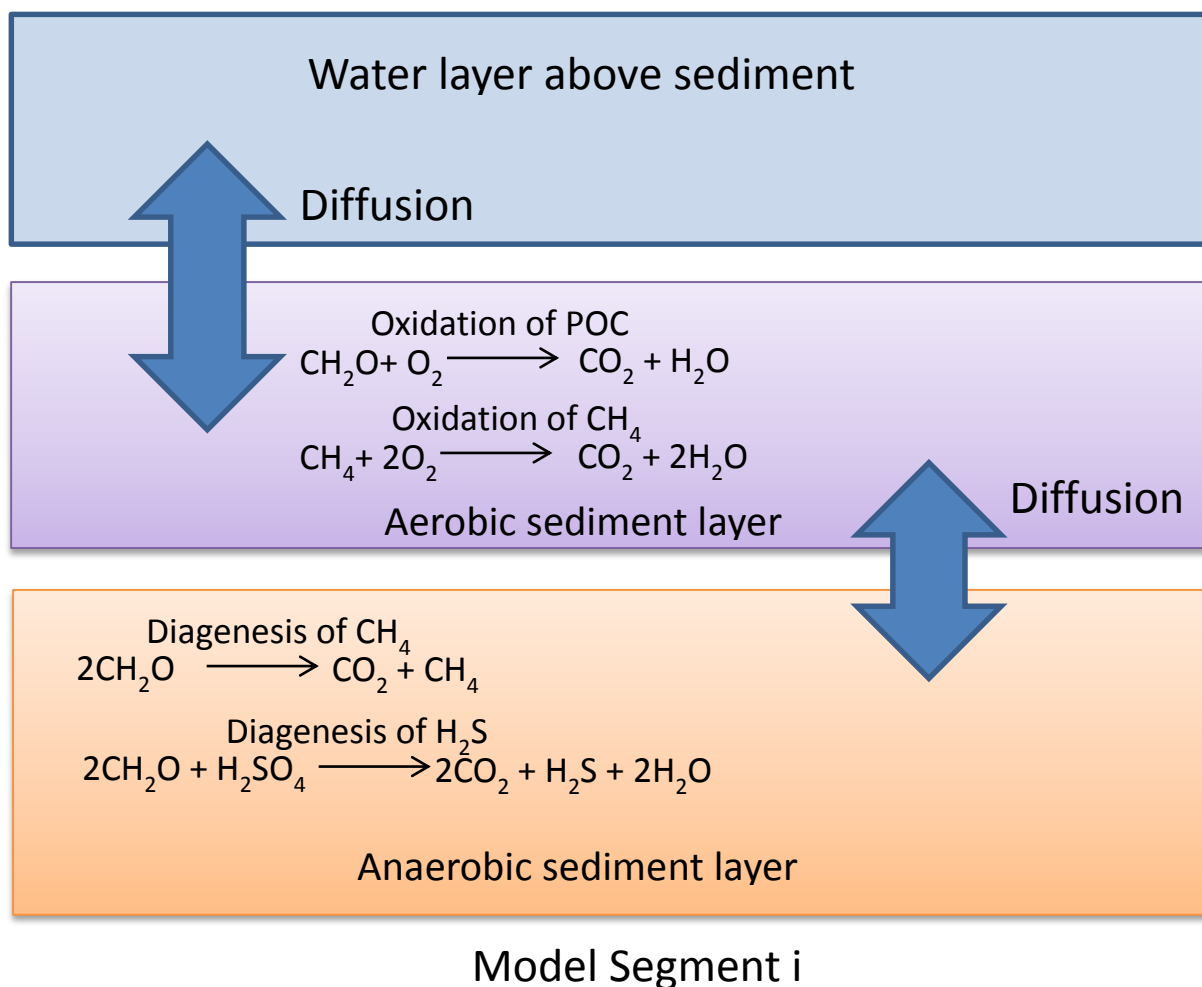
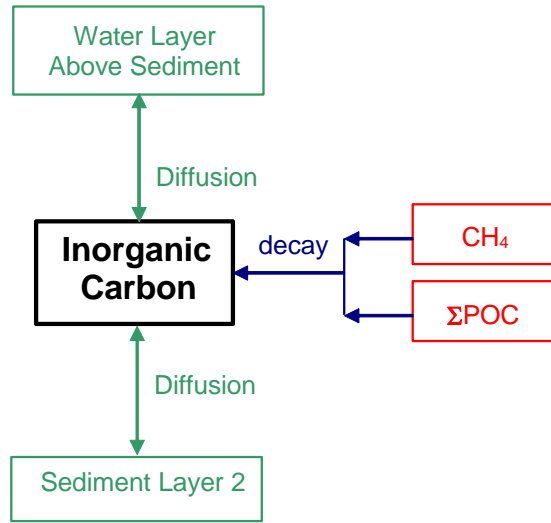
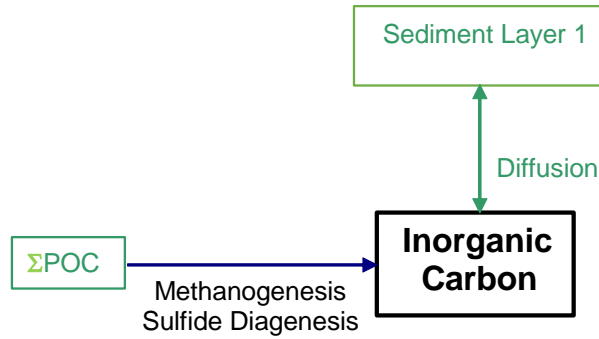


Figure 6 Schematic of sediment inorganic carbon model.



**Figure 7 Internal flux between inorganic carbon within the aerobic sediment layer 1 and other compartments**



**Figure 8 Internal flux between inorganic carbon within the anaerobic sediment layer 2 and other compartments**

The rate equation for total inorganic carbon (TIC) in the aerobic sediment layer 1 is:

$$S_{TIC1} = \underbrace{\sum k_{POC1} \gamma_{POC} \Phi_{POC}}_{\text{POC decay}} + \underbrace{k_{CH41} \gamma_{CH4} \Phi_{CH4}}_{\text{CH4 decay}}$$

where:

$\gamma_{POC}$  = particulate organic carbon temperature rate multiplier

$\gamma_{CH4}$  = methane temperature rate multiplier

$k_{POC1}$  = POC decay rate in layer 1,  $sec^{-1}$   
 $k_{CH41}$  = methane decay rate in layer 1,  $sec^{-1}$   
 $k_{POCm2}$  = methanogenesis rate in layer 2,  $sec^{-1}$   
 $k_{POCs2}$  = sulfide diagenesis rate in layer 2,  $sec^{-1}$   
 $\Phi_{POC}$  = particulate organic carbon concentration,  $g\ m^{-3}$   
 $\Phi_{CH4}$  = methane concentration,  $g\ m^{-3}$

The rate equation for TIC in the anaerobic sediment layer 2 is:

$$S_{TIC2} = \underbrace{\sum k_{POCm2} \gamma_{POC} \Phi_{POC}}_{\text{Methanogenesis}} + \underbrace{k_{POCs2} \gamma_{POC} \Phi_{POC}}_{\text{Sulfide Diagenesis}}$$

The mass balances for layer 1 and layer 2 are:

$$H_1 \frac{d\Phi_{TIC1}}{dt} = -K_{L01}(\Phi_{TIC1} - \Phi_{TIC0}) + K_{L12}(\Phi_{TIC2} - \Phi_{TIC1}) + H_1 S_{TIC1}$$

$$H_2 \frac{d\Phi_{TIC2}}{dt} = -K_{L12}(\Phi_{TIC2} - \Phi_{TIC1}) + H_2 S_{TIC2}$$

where

$\Phi_{TIC1}$  = total inorganic carbon concentration in layer 1,  $g\ m^{-3}$   
 $\Phi_{TIC2}$  = total inorganic carbon concentration in layer 2,  $g\ m^{-3}$   
 $\Phi_{TIC0}$  = total inorganic carbon concentration in water column,  $g\ m^{-3}$   
 $H_1$  = height of layer 1,  $m$   
 $H_2$  = height of layer 2,  $m$   
 $K_{L01}$  = mass transfer coefficient between water column and layer 1,  $m\ s^{-1}$   
 $K_{L12}$  = mass transfer coefficient between layer 1 and layer 2,  $m\ s^{-1}$

The mass transfer coefficient  $K_{L12}$  is related to the diffusion coefficient  $D$  using

$$K_{L12} = \frac{D}{\Delta z} = \frac{D}{\frac{1}{2}(H_1 + H_2)}$$

The implicit finite difference scheme for layer 1 is

$$H_1 \frac{\Phi_{TIC1}^{t+\Delta t} - \Phi_{TIC1}^t}{\Delta t} = -K_{L01}(\Phi_{TIC1}^{t+\Delta t} - \Phi_{TIC0}) + K_{L12}(\Phi_{TIC2}^{t+\Delta t} - \Phi_{TIC1}^{t+\Delta t}) + H_1 S_{TIC1}$$

Rearranging

$$\left(-\frac{H_1}{\Delta t} - K_{L01} - K_{L12}\right) \Phi_{TIC1}^{t+\Delta t} + K_{L12} \Phi_{TIC2}^{t+\Delta t} = -H_1 S_{TIC1} - \frac{H_1}{\Delta t} \Phi_{TIC1}^t - K_{L01} \Phi_{TIC0}$$

And the finite difference scheme for layer 2

$$H_2 \frac{\Phi_{TIC2}^{t+\Delta t} - \Phi_{TIC2}^t}{\Delta t} = -K_{L12}(\Phi_{TIC2}^{t+\Delta t} - \Phi_{TIC1}^{t+\Delta t}) + H_2 S_{TIC2}$$

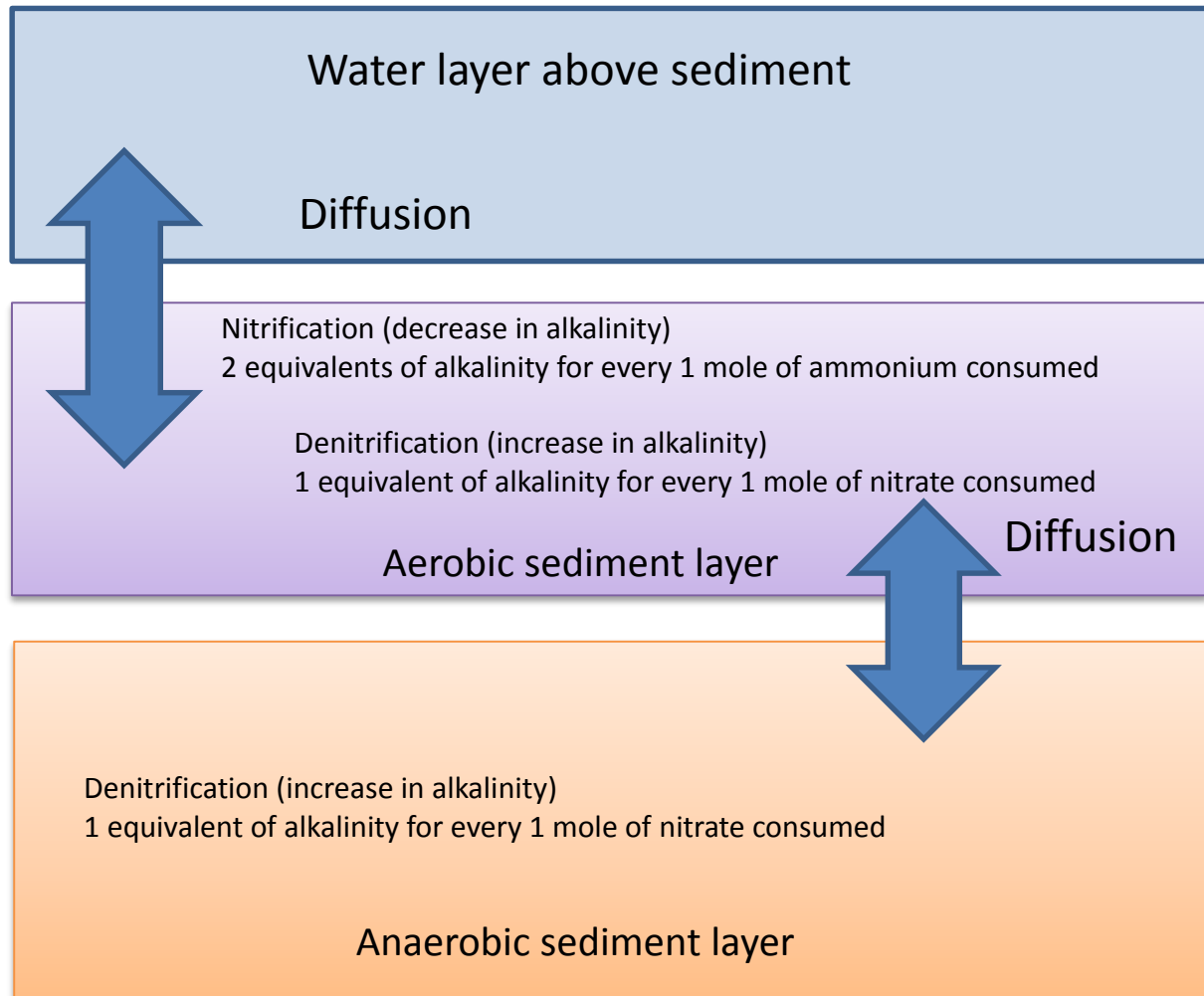
Rearranging

$$K_{L12} \Phi_{TIC1}^{t+\Delta t} + \left(-\frac{H_2}{\Delta t} - K_{L12}\right) \Phi_{TIC2}^{t+\Delta t} = -H_2 S_{TIC2} - \frac{H_2}{\Delta t} \Phi_{TIC2}^t$$



## Sediment Alkalinity

Sources and sinks for non-conservative sediment alkalinity model is shown in Figure 9. Alkalinity is in units of mg/l as  $\text{CaCO}_3$ .



### Model Segment i

Figure 9. Sources and sinks of the sediment alkalinity model.

The rate equation for alkalinity in the aerobic sediment layer 1 is:

$$S_{ALK1} = - \underbrace{\left( \frac{2 \text{ equivalents alkalinity}}{1 \text{ mole ammonium nitrified}} \right) k_{NH4} \gamma_{NH4} \Phi_{NH4}}_{\text{nitrification}} + \underbrace{\left( \frac{1 \text{ equivalent alkalinity}}{1 \text{ mole nitrate denitrified}} \right) k_{NOx} \gamma_{NOx1} \Phi_{NOx}}_{\text{denitrification}}$$

where:

$\gamma_{NOx}$  = denitrification temperature rate multiplier

$\gamma_{NH4}$  = nitrification temperature rate multiplier

$k_{NOx1}$  = denitrification rate in aerobic layer,  $\text{sec}^{-1}$

$k_{NH4}$  = nitrification rate,  $\text{sec}^{-1}$

$\Phi_{NOx}$  = nitrate-nitrite concentration,  $\text{g m}^{-3}$

$\Phi_{NH4}$  = ammonium concentration,  $\text{g m}^{-3}$

The rate equation for alkalinity in the anaerobic sediment layer 2 is:

$$S_{ALK2} = \underbrace{\left( \frac{1 \text{ equivalent alkalinity}}{1 \text{ mole nitrate denitrified}} \right) k_{NOx} \gamma_{NOx} \Phi_{NOx}}_{\text{denitrification}}$$

where

$k_{NOx2}$  = denitrification rate in anaerobic layer,  $\text{sec}^{-1}$

The mass balances for layer 1 and layer 2 are:

$$H_1 \frac{d\Phi_{ALK1}}{dt} = -K_{L01}(\Phi_{ALK1} - \Phi_{ALK0}) + K_{L12}(\Phi_{ALK2} - \Phi_{ALK1}) + H_1 S_{ALK1}$$

$$H_2 \frac{d\Phi_{ALK2}}{dt} = -K_{L12}(\Phi_{ALK2} - \Phi_{ALK1}) + H_2 S_{ALK2}$$

where

$\Phi_{ALK1}$  = alkalinity concentration in layer 1,  $\text{g m}^{-3}$

$\Phi_{ALK2}$  = alkalinity concentration in layer 2,  $\text{g m}^{-3}$

$\Phi_{ALK0}$  = alkalinity concentration in water column,  $\text{g m}^{-3}$

$H_1$  = height of layer 1,  $\text{m}$

$H_2$  = height of layer 2,  $\text{m}$

$K_{L01}$  = mass transfer coefficient between water column and layer 1,  $\text{m s}^{-1}$

$K_{L12}$  = mass transfer coefficient between layer 1 and layer 2,  $\text{m s}^{-1}$

The implicit finite difference scheme of alkalinity is equivalent to that used for inorganic carbon.

## Sediment Temperature

A schematic of the sediment temperature model is shown in Figure 10.

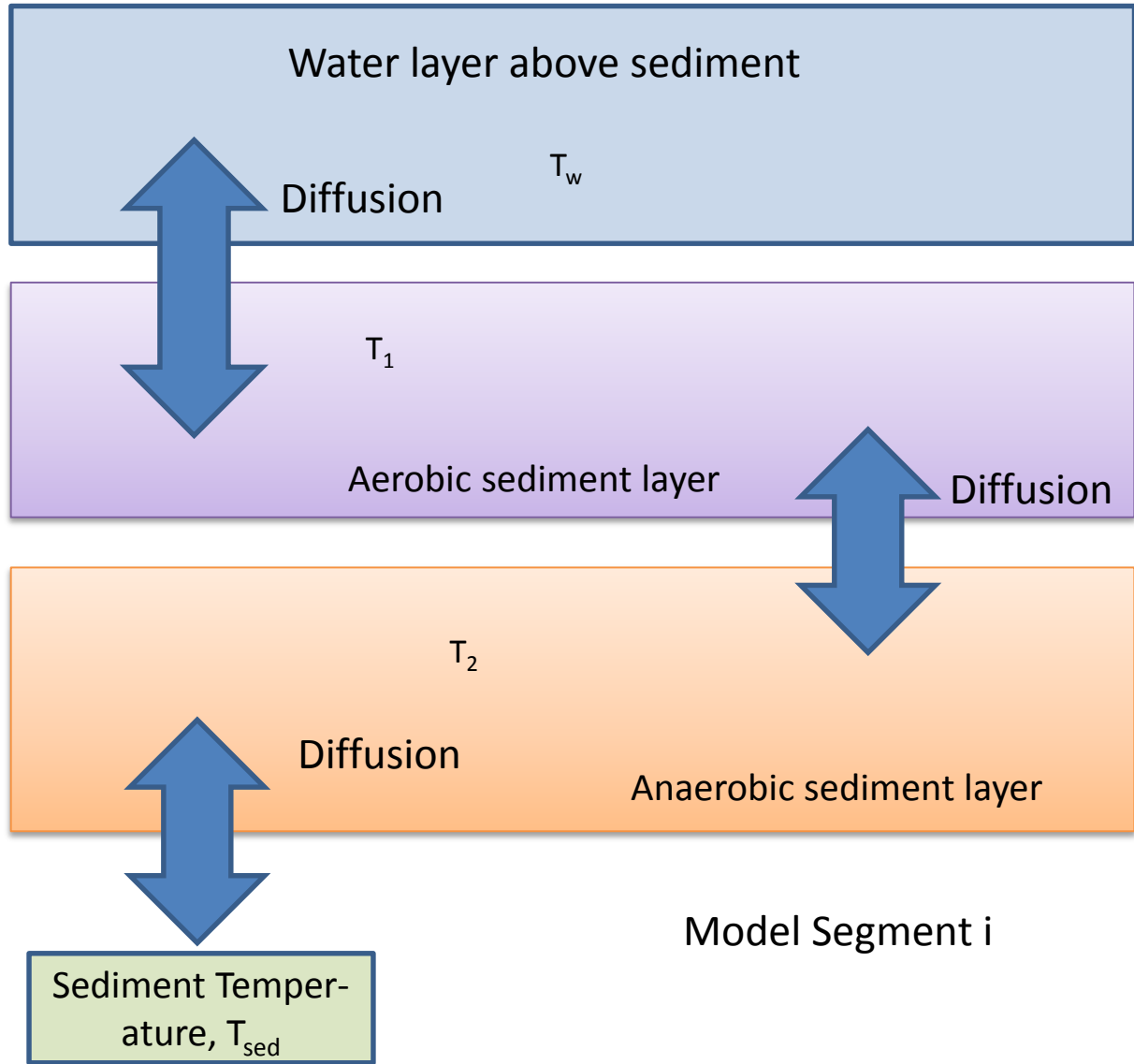


Figure 10. Schematic of sediment temperature model.

The heat balances for the aerobic layer 1 and anaerobic layer 2 are:

$$\rho C_p H_1 \frac{dT_1}{dt} = -K_{L01} \rho C_p (T_1 - T_0) + K_{L12} \rho C_p (T_2 - T_1)$$

$$\rho C_p H_2 \frac{dT_2}{dt} = -K_{L12} \rho C_p (T_2 - T_1) + K_{sw} (T_{sed} - T_2)$$

where

$T_1$  = temperature in layer 1, °C

$T_2$  = temperature in layer 2, °C

$T_0$  = temperature in water column, °C

$T_{sed}$  = temperature of sediments below anaerobic layer, °C

$H_1$  = height of layer 1, m

$H_2$  = height of layer 2, m

$K_{L01}$  = heat transfer coefficient between water column and layer 1,  $m s^{-1}$

$K_{L12}$  = heat transfer coefficient between layer 1 and layer 2,  $m s^{-1}$

$K_{sw}$  = coefficient of sediment heat exchange between anaerobic layer and sediments below anaerobic layer,  $W m^{-2} °C^{-1}$

$\rho$  = water density,  $g m^{-3}$

$C_p$  = water density,  $J g^{-1} °C^{-1}$

The implicit finite difference scheme for layer 1 is

$$\rho C_p H_1 \frac{T_1^{t+\Delta t} - T_1^t}{\Delta t} = -K_{L01} \rho C_p (T_1^{t+\Delta t} - T_0) + K_{L12} \rho C_p (T_2^{t+\Delta t} - T_1^{t+\Delta t})$$

Rearranging and cancelling out  $\rho C_p$

$$\left( -\frac{H_1}{\Delta t} - K_{L01} - K_{L12} \right) T_1^{t+\Delta t} + K_{L12} T_2^{t+\Delta t} = -\frac{H_1}{\Delta t} T_1^t - K_{L01} T_0$$

And the finite difference scheme for layer 2

$$\rho C_p H_2 \frac{T_2^{t+\Delta t} - T_2^t}{\Delta t} = -K_{L12} \rho C_p (T_2^{t+\Delta t} - T_1^{t+\Delta t}) + K_{sw} (T_{sed} - T_2^{t+\Delta t})$$

Rearranging

$$K_{L12} \rho C_p T_1^{t+\Delta t} + \left( -\frac{\rho C_p H_2}{\Delta t} - \rho C_p K_{L12} + K_{sw} \right) T_2^{t+\Delta t} = -\frac{\rho C_p H_2}{\Delta t} T_2^t - K_{sw} T_{sed}$$

## Metal Complexation and Diagenesis

### Ferrous Iron Fe(II)

Iron is modeled using two constituents: iron oxyhydroxide, FeOOH(s), and ferrous iron Fe(II). FeOOH(s) is very insoluble and is modeled as a particulate whereas Fe(II) is more soluble. Figure 11 illustrates the iron model within the water column and sediments.

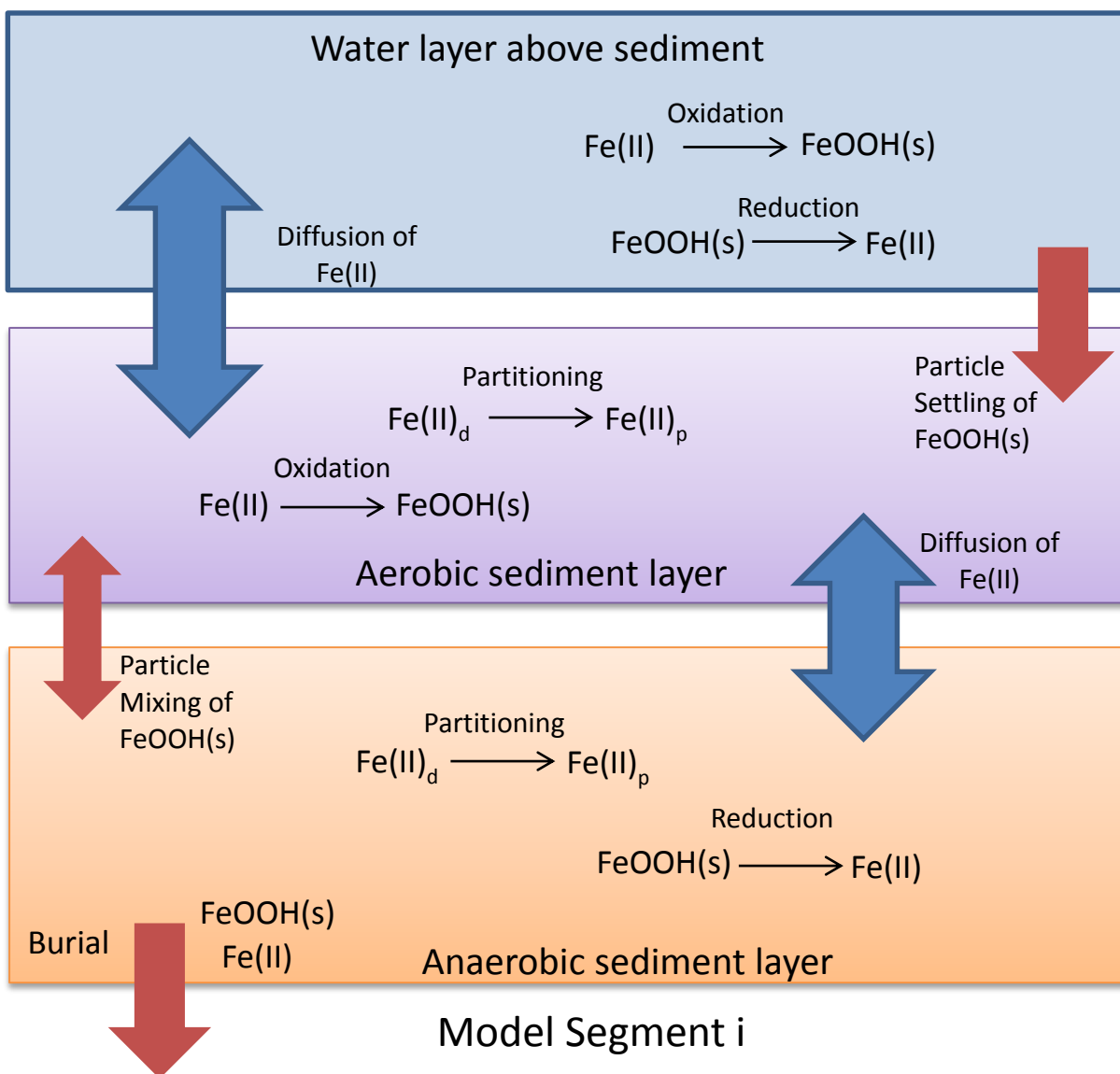


Figure 11. Schematic of iron model (Ditoro, 2001).

The modeling of ferrous iron in the water column was added to CE-QUAL-W2. The rate equation in the water column is:

$$S_{Fe(II)} = \underbrace{-k_{Fe(II)0} \Phi_{DO} 10^{2(pH-7)} \Phi_{Fe(II)}}_{\text{Oxidation}} + \underbrace{k_{FeOOH} \left( \frac{K_{FeOOH}}{K_{FeOOH} + \Phi_{DO}} \right) \Phi_{FeOOH}}_{\text{Reduction}}$$

Where

$k_{FeOOH}$  = reduction rate in water column,  $sec^{-1}$

$k_{Fe(II)0}$  = oxidation rate in water column,  $sec^{-1}(g\ m^{-3})^{-1}$

$K_{FeOOH}$  = half saturation constant for oxygen for this reaction,  $g\ m^{-3}$

$\Phi_{DO}$  = dissolved oxygen concentration,  $g\ m^{-3}$

$\Phi_{Fe(II)}$  = ferrous iron concentration,  $g\ m^{-3}$

$\Phi_{FeOOH}$  = iron oxyhydroxide concentration,  $g\ m^{-3}$

$pH$  = pH in water column

The rate equation for ferrous iron in sediment layer 1 is:

$$S_{Fe(II)1} = \underbrace{-k_{Fe(II)1} \Phi_{DO} 10^{2(pH1-7)} f_d \Phi_{Fe(II)1}}_{\text{Oxidation}}$$

where:

$f_d$  = dissolved fraction of ferrous iron

$k_{Fe(II)1}$  = ferrous iron oxidation rate in layer 1,  $sec^{-1}(g\ m^{-3})^{-1}$

$\Phi_{DO}$  = dissolved oxygen concentration,  $g\ m^{-3}$

$\Phi_{Fe(II)}$  = ferrous iron concentration,  $g\ m^{-3}$

$pH1$  = pH in layer 1

The rate equation for ferrous iron in sediment layer 2 is:

$$S_{Fe(II)2} = \underbrace{k_{FeOOH2} \Phi_{FeOOH}}_{\text{Reduction}}$$

$k_{FeOOH2}$  = ferrous iron reduction rate in layer 2,  $sec^{-1}$

$\Phi_{FeOOH}$  = iron oxyhydroxide concentration,  $g\ m^{-3}$

Mass balances for the aerobic layer 1 and anaerobic layer 2 are:

$$H_1 \frac{d\Phi_{Fe(II)1}}{dt} = -K_{L01}(f_d \Phi_{Fe(II)1} - \Phi_{Fe(II)0}) + K_{L12}(f_d \Phi_{Fe(II)2} - f_d \Phi_{Fe(II)1}) \\ + w_{12}(f_p \Phi_{Fe(II)2} - f_p \Phi_{Fe(II)1}) - w_2 \Phi_{Fe(II)1} + H_1 S_{Fe(II)1}$$

$$H_2 \frac{d\Phi_{Fe(II)2}}{dt} = -K_{L12}(f_d \Phi_{Fe(II)2} - f_d \Phi_{Fe(II)1}) - w_{12}(f_p \Phi_{Fe(II)2} - f_p \Phi_{Fe(II)1}) \\ + w_2(\Phi_{Fe(II)1} - \Phi_{Fe(II)2}) + H_2 S_{Fe(II)2}$$

where

$\Phi_{Fe(II)0}$  = ferrous iron concentration in water column,  $g\ m^{-3}$

$H_1$  = height of layer 1,  $m$   
 $H_2$  = height of layer 2,  $m$   
 $K_{L01}$  = mass transfer coefficient between water column and layer 1,  $m\ s^{-1}$   
 $K_{L12}$  = mass transfer coefficient between layer 1 and layer 2,  $m\ s^{-1}$   
 $f_d$  = dissolved fraction of ferrous iron  
 $f_p$  = particulate fraction of ferrous iron  
 $w_{12}$  = particle mixing velocity between layer 1 and layer 2,  $m\ s^{-1}$   
 $w_2$  = burial velocity,  $m\ s^{-1}$

The implicit finite difference scheme for layer 1 is

$$\begin{aligned}
 H_1 \frac{\Phi_{Fe(II)1}^{t+\Delta t} - \Phi_{Fe(II)1}^t}{\Delta t} &= -K_{L01}(f_d \Phi_{Fe(II)1}^{t+\Delta t} - \Phi_{Fe(II)0}) + K_{L12}(f_d \Phi_{Fe(II)2}^{t+\Delta t} - f_d \Phi_{Fe(II)1}^{t+\Delta t}) \\
 &+ w_{12}(f_p \Phi_{Fe(II)2}^{t+\Delta t} - f_p \Phi_{Fe(II)1}^{t+\Delta t}) - w_2 \Phi_{Fe(II)1}^{t+\Delta t} \\
 &- H_1 k_{Fe(II)1} \Phi_{DO} 10^{2(pH1-7)} f_d \Phi_{Fe(II)1}^{t+\Delta t}
 \end{aligned}$$

Rearranging

$$\begin{aligned}
 \left( -\frac{H_1}{\Delta t} - f_d K_{L01} - f_d K_{L12} - w_{12} f_p - w_2 - H_1 k_{Fe(II)1} \Phi_{DO} 10^{2(pH1-7)} f_d \right) \Phi_{Fe(II)1}^{t+\Delta t} \\
 + (K_{L12} f_d + w_{12} f_p) \Phi_{Fe(II)2}^{t+\Delta t} = -\frac{H_1}{\Delta t} \Phi_{Fe(II)1}^t - K_{L01} \Phi_{Fe(II)0}
 \end{aligned}$$

And the finite difference scheme for layer 2

$$\begin{aligned}
 H_2 \frac{\Phi_{Fe(II)2}^{t+\Delta t} - \Phi_{Fe(II)2}^t}{\Delta t} &= -K_{L12}(f_d \Phi_{Fe(II)2}^{t+\Delta t} - f_d \Phi_{Fe(II)1}^{t+\Delta t}) - w_{12}(f_p \Phi_{Fe(II)2}^{t+\Delta t} - f_p \Phi_{Fe(II)1}^{t+\Delta t}) \\
 &+ w_2 (\Phi_{Fe(II)1}^{t+\Delta t} - \Phi_{Fe(II)2}^{t+\Delta t}) + H_2 S_{Fe(II)2}
 \end{aligned}$$

Rearranging

$$\begin{aligned}
 (f_d K_{L12} + f_p w_{12} + w_2) \Phi_{Fe(II)1}^{t+\Delta t} + \left( -\frac{H_2}{\Delta t} - f_d K_{L12} - f_p w_{12} - w_2 \right) \Phi_{Fe(II)2}^{t+\Delta t} \\
 = -H_2 S_{Fe(II)2} - \frac{H_2}{\Delta t} \Phi_{Fe(II)2}^t
 \end{aligned}$$

The fractions associated with dissolved and particulate forms can be calculated with (Chapra, 1997):

$$\begin{aligned}
 f_d &= \left( \frac{1}{\varphi + K_{dFe}(1 - \varphi)\rho} \right) \\
 f_p &= \left( \frac{K_{dFe}(1 - \varphi)\rho}{\varphi + K_{dFe}(1 - \varphi)\rho} \right)
 \end{aligned}$$

Where

$f_d$  = dissolved fraction of ferrous iron

$f_p$  = particulate fraction of ferrous iron  
 $\varphi$  = sediment porosity  
 $\rho$  = sediment density,  $g\ m^{-3}$   
 $K_{dFe}$  = ferrous sorption coefficient,  $m^3\ g^{-1}$

## Iron Oxyhydroxide FeOOH(s)

The rate equation in the water column for iron oxyhydroxide is:

$$S_{FeOOH} = \underbrace{k_{Fe(II)0} \Phi_{DO} 10^{2(pH-7)} \Phi_{Fe(II)}}_{\text{Oxidation}} - \underbrace{k_{FeOOH} \left( \frac{K_{FeOOH}}{K_{FeOOH} + \Phi_{DO}} \right) \Phi_{FeOOH}}_{\text{Reduction}}$$

where

$k_{FeOOH}$  = reduction rate in water column,  $sec^{-1}$   
 $k_{Fe(II)0}$  = oxidation rate in water column,  $sec^{-1}(g\ m^{-3})^{-1}$   
 $K_{FeOOH}$  = half saturation constant for oxygen for this reaction,  $g\ m^{-3}$   
 $\Phi_{DO}$  = dissolved oxygen concentration,  $g\ m^{-3}$   
 $\Phi_{FeOOH}$  = iron oxyhydroxide concentration,  $g\ m^{-3}$   
 $\Phi_{Fe(II)}$  = ferrous iron concentration,  $g\ m^{-3}$   
 $pH$  = pH in water column

The rate equation for iron oxyhydroxide in the aerobic sediment layer 1 is:

$$S_{FeOOH1} = \underbrace{k_{Fe(II)1} \Phi_{DO} 10^{2(pH1-7)} f_d \Phi_{Fe(II)1}}_{\text{Oxidation}}$$

where

$f_d$  = dissolved fraction of ferrous iron  
 $k_{Fe(II)1}$  = ferrous iron oxidation rate in layer 1,  $sec^{-1}(g\ m^{-3})^{-1}$   
 $\Phi_{DO}$  = dissolved oxygen concentration,  $g\ m^{-3}$   
 $\Phi_{Fe(II)}$  = ferrous iron concentration,  $g\ m^{-3}$   
 $pH1$  = pH in layer 1

The rate equation for iron oxyhydroxide in the anaerobic sediment layer 2 is:

$$S_{FeOOH2} = \underbrace{-k_{FeOOH2} \Phi_{FeOOH}}_{\text{Reduction}}$$

where

$k_{FeOOH2}$  = ferrous iron reduction rate in layer 2,  $sec^{-1}$   
 $\Phi_{FeOOH}$  = iron oxyhydroxide concentration,  $g\ m^{-3}$

Mass balances for layer 1 and layer 2 are:

$$H_1 \frac{d\Phi_{FeOOH1}}{dt} = w_{12}(\Phi_{FeOOH2} - \Phi_{FeOOH1}) - w_2 \Phi_{FeOOH1} + w_1 \Phi_{FeOOH0} + H_1 S_{FeOOH1}$$



$$H_2 \frac{d\Phi_{FeOOH2}}{dt} = -w_{12}(\Phi_{FeOOH2} - \Phi_{FeOOH1}) + w_2(\Phi_{FeOOH1} - \Phi_{FeOOH2}) + H_2 S_{FeOOH2}$$

where

$\Phi_{FeOOH0}$  = iron oxyhydroxide concentration in water column,  $g\ m^{-3}$

$H_1$  = height of layer 1,  $m$

$H_2$  = height of layer 2,  $m$

$w_1$  = particle settling velocity,  $m\ s^{-1}$

$w_{12}$  = particle mixing velocity between layer 1 and layer 2,  $m\ s^{-1}$

$w_2$  = burial velocity,  $m\ s^{-1}$

The implicit finite difference scheme for layer 1 is

$$\begin{aligned} H_1 \frac{\Phi_{FeOOH1}^{t+\Delta t} - \Phi_{FeOOH1}^t}{\Delta t} &= w_{12}(\Phi_{FeOOH2}^{t+\Delta t} - \Phi_{FeOOH1}^{t+\Delta t}) - w_2 \Phi_{FeOOH1}^{t+\Delta t} + w_1 \Phi_{FeOOH0} \\ &\quad + H_1 k_{Fe(II)1} \Phi_{DO} 10^{2(pH1-7)} f_d \Phi_{Fe(II)1}^t \end{aligned}$$

Rearranging

$$\begin{aligned} \left( -\frac{H_1}{\Delta t} - w_{12} - w_2 \right) \Phi_{FeOOH1}^{t+\Delta t} + w_{12} \Phi_{FeOOH2}^{t+\Delta t} \\ = -\frac{H_1}{\Delta t} \Phi_{FeOOH1}^t - w_1 \Phi_{FeOOH0} - H_1 k_{Fe(II)1} \Phi_{DO} 10^{2(pH1-7)} f_d \Phi_{Fe(II)1}^t \end{aligned}$$

And the finite difference scheme for layer 2

$$\begin{aligned} H_2 \frac{\Phi_{FeOOH2}^{t+\Delta t} - \Phi_{FeOOH2}^t}{\Delta t} &= -w_{12}(\Phi_{FeOOH2}^{t+\Delta t} - \Phi_{FeOOH1}^{t+\Delta t}) + w_2(\Phi_{FeOOH1}^{t+\Delta t} - \Phi_{FeOOH2}^{t+\Delta t}) \\ &\quad - H_2 k_{FeOOH} \Phi_{FeOOH2}^{t+\Delta t} \end{aligned}$$

Rearranging

$$(w_{12} + w_2) \Phi_{FeOOH1}^{t+\Delta t} + \left( -\frac{H_2}{\Delta t} - w_{12} - w_2 - H_2 k_{FeOOH} \right) \Phi_{FeOOH2}^{t+\Delta t} = -\frac{H_2}{\Delta t} \Phi_{FeOOH2}^t$$

## Manganese Mn(II)

The manganese model within the water column and sediments is illustrated in Figure 11.

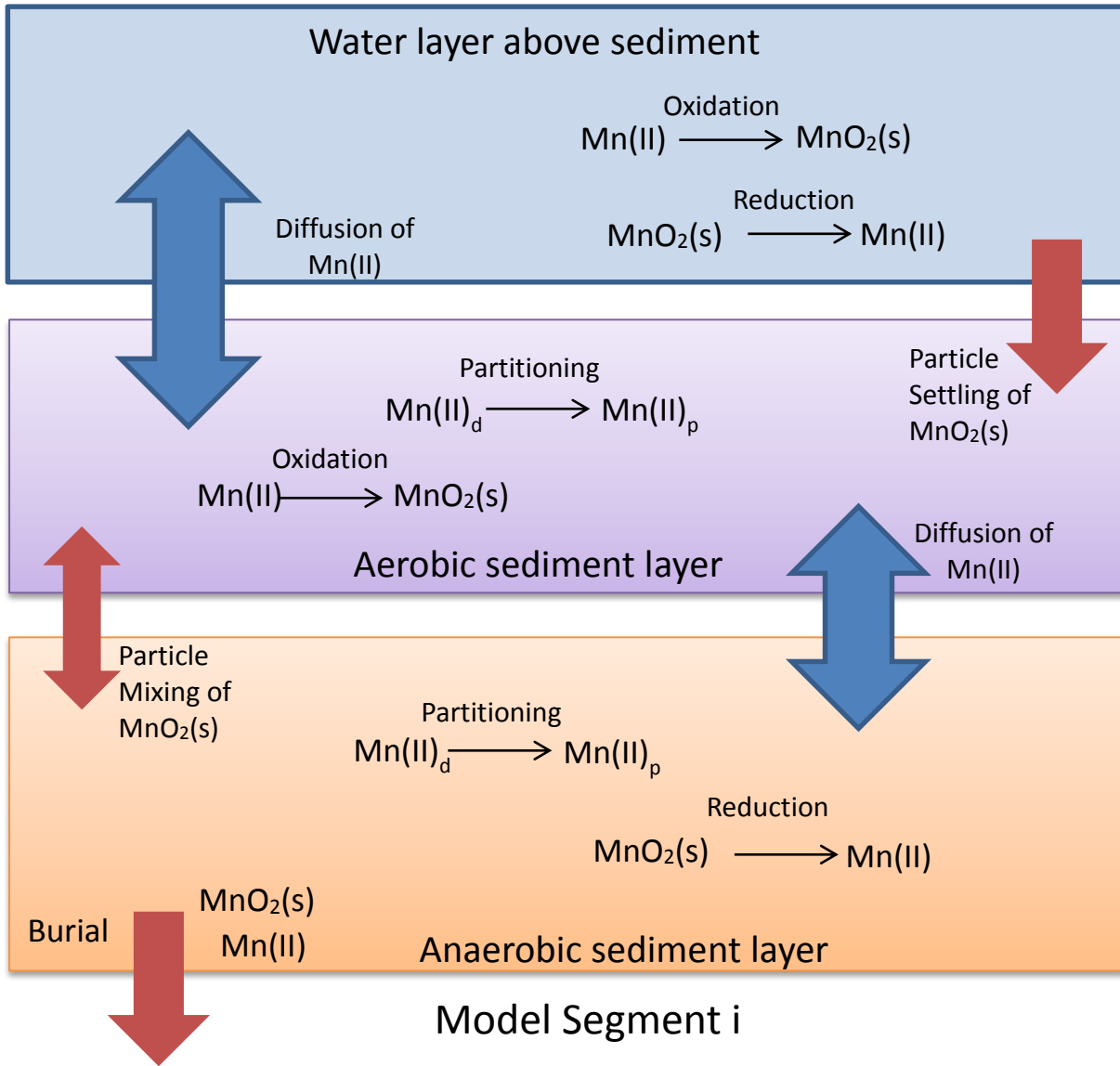


Figure 12. Schematic of manganese model (Ditoro, 2001).

The following rate equation is used to model ionic divalent manganese Mn(II) in the water column is:

$$S_{Mn(II)} = \underbrace{-k_{Mn(II)0} \Phi_{DO} 10^{2(pH-7)} \Phi_{Mn(II)}}_{\text{Oxidation}} + \underbrace{k_{MnO_2} \left( \frac{K_{MnO_2}}{K_{MnO_2} + \Phi_{DO}} \right) \Phi_{MnO_2}}_{\text{Reduction}}$$

Where

$k_{MnO_2}$  = reduction rate in water column,  $sec^{-1}$

$k_{Mn(II)0}$  = oxidation rate in water column,  $sec^{-1}(g\ m^{-3})^{-1}$

$K_{MnO_2}$  = half saturation constant for oxygen for this reaction,  $g\ m^{-3}$

$\Phi_{DO}$  = dissolved oxygen concentration,  $g\ m^{-3}$

$\Phi_{Mn(II)}$  = Mn(II) concentration,  $g\ m^{-3}$

$\Phi_{MnO_2}$  = manganese dioxide concentration,  $g\ m^{-3}$

$pH$  = pH in water column

The rate equation for Mn(II) in the aerobic sediment layer 1 is:

$$S_{Mn(II)1} = \underbrace{-k_{Mn(II)1} \Phi_{DO} 10^{2(pH1-7)} f_d \Phi_{Mn(II)1}}_{\text{Oxidation}}$$

where:

$f_d$  = dissolved fraction of Mn(II)

$k_{Mn(II)1}$  = Mn(II) oxidation rate in layer 1,  $sec^{-1}(g\ m^{-3})^{-1}$

$\Phi_{DO}$  = dissolved oxygen concentration,  $g\ m^{-3}$

$\Phi_{Mn(II)1}$  = Mn(II) concentration,  $g\ m^{-3}$

$pH1$  = pH in layer 1

The rate equation for manganese dioxide in the anaerobic sediment layer 2 is:

$$S_{Mn(II)2} = \underbrace{k_{MnO_2} \Phi_{MnO_2}}_{\text{Reduction}}$$

where:

$k_{MnO_2}$  = manganese dioxide reduction rate in layer 2,  $sec^{-1}$

$\Phi_{MnO_2}$  = manganese dioxide concentration,  $g\ m^{-3}$

Mass balances for layer 1 and layer 2 are then:

$$\begin{aligned} H_1 \frac{d\Phi_{Mn(II)1}}{dt} &= -K_{L01}(f_d \Phi_{Mn(II)1} - \Phi_{Mn(II)0}) + K_{L12}(f_d \Phi_{Mn(II)2} - f_d \Phi_{Mn(II)1}) \\ &\quad + w_{12}(f_p \Phi_{Mn(II)2} - f_p \Phi_{Mn(II)1}) - w_2 \Phi_{Mn(II)1} + H_1 S_{Mn(II)1} \\ H_2 \frac{d\Phi_{Mn(II)2}}{dt} &= -K_{L12}(f_d \Phi_{Mn(II)2} - f_d \Phi_{Mn(II)1}) - w_{12}(f_p \Phi_{Mn(II)2} - f_p \Phi_{Mn(II)1}) \\ &\quad + w_2(\Phi_{Mn(II)1} - \Phi_{Mn(II)2}) + H_2 S_{Mn(II)2} \end{aligned}$$

where:

$\Phi_{Mn(II)0}$  = Mn(II) concentration in water column,  $g\ m^{-3}$

$H_1$  = height of layer 1,  $m$

$H_2$  = height of layer 2,  $m$

$K_{L01}$  = mass transfer coefficient between water column and layer 1,  $m\ s^{-1}$

$K_{L12}$  = mass transfer coefficient between layer 1 and layer 2,  $m\ s^{-1}$

$f_d$  = dissolved fraction of Mn(II)

$f_p$  = particulate fraction of Mn(II)

$w_{12}$  = particle mixing velocity between layer 1 and layer 2,  $m\ s^{-1}$

$w_2$  = burial velocity,  $m\ s^{-1}$

The implicit finite difference scheme for layer 1 is

$$\begin{aligned} H_1 \frac{\Phi_{Mn(II)1}^{t+\Delta t} - \Phi_{Mn(II)1}^t}{\Delta t} &= -K_{L01}(f_d \Phi_{Mn(II)1}^{t+\Delta t} - \Phi_{Mn(II)0}) + K_{L12}(f_d \Phi_{Mn(II)2}^{t+\Delta t} - f_d \Phi_{Mn(II)1}^{t+\Delta t}) \\ &\quad + w_{12}(f_p \Phi_{Mn(II)2}^{t+\Delta t} - f_p \Phi_{Mn(II)1}^{t+\Delta t}) - w_2 \Phi_{Mn(II)1}^{t+\Delta t} \\ &\quad - H_1 k_{Mn(II)1} \Phi_{DO} 10^{2(pH1-7)} f_d \Phi_{Mn(II)1}^{t+\Delta t} \end{aligned}$$

Rearranging

$$\left(-\frac{H_1}{\Delta t} - f_d K_{L01} - f_d K_{L12} - w_{12} f_p - w_2 - H_1 k_{Mn(II)1} \Phi_{DO} 10^{2(pH-7)} f_d\right) \Phi_{Mn(II)1}^{t+\Delta t} + (K_{L12} f_d + w_{12} f_p) \Phi_{Mn(II)2}^{t+\Delta t} = -\frac{H_1}{\Delta t} \Phi_{Mn(II)1}^t - K_{L01} \Phi_{Mn(II)0}$$

And the finite difference scheme for layer 2

$$\begin{aligned} H_2 \frac{\Phi_{Mn(II)2}^{t+\Delta t} - \Phi_{Mn(II)2}^t}{\Delta t} &= -K_{L12} (f_d \Phi_{Mn(II)2}^{t+\Delta t} - f_d \Phi_{Mn(II)1}^{t+\Delta t}) - w_{12} (f_p \Phi_{Mn(II)2}^{t+\Delta t} - f_p \Phi_{Mn(II)1}^{t+\Delta t}) \\ &+ w_2 (\Phi_{Mn(II)1}^{t+\Delta t} - \Phi_{Mn(II)2}^{t+\Delta t}) + H_2 S_{Mn(II)2} \end{aligned}$$

Rearranging

$$\begin{aligned} (f_d K_{L12} + f_p w_{12} + w_2) \Phi_{Mn(II)1}^{t+\Delta t} + \left(-\frac{H_2}{\Delta t} - f_d K_{L12} - f_p w_{12} - w_2\right) \Phi_{Mn(II)2}^{t+\Delta t} \\ = -H_2 S_{Mn(II)2} - \frac{H_2}{\Delta t} \Phi_{Mn(II)2}^t \end{aligned}$$

The fractions associated with dissolved and particulate forms can be calculated with (Chapra, 1997):

$$\begin{aligned} f_d &= \left( \frac{1}{\varphi + K_{dMn}(1 - \varphi)\rho} \right) \\ f_p &= \left( \frac{K_{dMn}(1 - \varphi)\rho}{\varphi + K_{dMn}(1 - \varphi)\rho} \right) \end{aligned}$$

where

$f_d$  = dissolved fraction of Mn(II)

$f_p$  = particulate fraction of Mn(II)

$\varphi$  = sediment porosity

$\rho$  = sediment density,  $g\ m^{-3}$

$K_{dp}$  = manganese sorption coefficient,  $m^3\ g^{-1}$

## Manganese Dioxide MnO<sub>2</sub>

The rate equation in the water column for manganese dioxide is:

$$S_{MnO_2} = \underbrace{k_{Mn(II)0} \Phi_{DO} 10^{2(pH-7)} \Phi_{Mn(II)}}_{\text{Oxidation}} - \underbrace{k_{MnO_2} \left( \frac{K_{MnO_2}}{K_{MnO_2} + \Phi_{DO}} \right) \Phi_{MnO_2}}_{\text{Reduction}}$$

where

$k_{MnO_2}$  = reduction rate in water column,  $sec^{-1}$

$k_{Mn(II)0}$  = oxidation rate in water column,  $sec^{-1}(g\ m^{-3})^{-1}$

$K_{MnO_2}$  = half saturation constant for oxygen for this reaction,  $g\ m^{-3}$

$\Phi_{DO}$  = dissolved oxygen concentration,  $g\ m^{-3}$

$\Phi_{Mn(II)}$  = Mn(II) concentration,  $g\ m^{-3}$

$\Phi_{MnO_2}$  = manganese dioxide concentration,  $g\ m^{-3}$

$pH=pH$  in water column

The rate equation for manganese dioxide in the aerobic sediment layer 1 is:

$$S_{MnO_2 1} = \underbrace{k_{Mn(II)1} \Phi_{DO} 10^{2(pH1-7)} f_d \Phi_{Mn(II)1}}_{\text{Oxidation}}$$

where

$f_d$  = dissolved fraction of Mn(II)

$k_{Mn(II)1}$  = Mn(II) oxidation rate in layer 1,  $sec^{-1}(g\ m^{-3})^{-1}$

$\Phi_{DO}$  = dissolved oxygen concentration,  $g\ m^{-3}$

$\Phi_{Mn(II)}$  = Mn(II) concentration,  $g\ m^{-3}$

$pH1$  = pH in layer 1

The rate equation for manganese dioxide in the anaerobic sediment layer 2 is:

$$S_{MnO_2 2} = \underbrace{-k_{MnO_2 2} \Phi_{MnO_2}}_{\text{Reduction}}$$

$k_{MnO_2 2}$  = manganese dioxide reduction rate in layer 2,  $sec^{-1}$

$\Phi_{MnO_2}$  = manganese dioxide concentration,  $g\ m^{-3}$

Mass balances for layer 1 and layer 2 are:

$$H_1 \frac{d\Phi_{MnO_2 1}}{dt} = w_{12}(\Phi_{MnO_2 2} - \Phi_{MnO_2 1}) - w_2 \Phi_{MnO_2 1} + w_1 \Phi_{MnO_2 0} + H_1 S_{MnO_2 1}$$

$$H_2 \frac{d\Phi_{MnO_2 2}}{dt} = -w_{12}(\Phi_{MnO_2 2} - \Phi_{MnO_2 1}) + w_2(\Phi_{MnO_2 1} - \Phi_{MnO_2 2}) + H_2 S_{MnO_2 2}$$

where

$\Phi_{MnO_2 0}$  = manganese concentration in water column,  $g\ m^{-3}$

$H_1$  = height of layer 1,  $m$

$H_2$  = height of layer 2,  $m$

$w_1$  = particle settling velocity,  $m\ s^{-1}$

$w_{12}$  = particle mixing velocity between layer 1 and layer 2,  $m\ s^{-1}$

$w_2$  = burial velocity,  $m\ s^{-1}$

The implicit finite difference scheme for layer 1 is

$$\begin{aligned} H_1 \frac{\Phi_{MnO_2 1}^{t+\Delta t} - \Phi_{MnO_2 1}^t}{\Delta t} &= w_{12}(\Phi_{MnO_2 2}^{t+\Delta t} - \Phi_{MnO_2 1}^{t+\Delta t}) - w_2 \Phi_{MnO_2 1}^{t+\Delta t} + w_1 \Phi_{MnO_2 0} \\ &+ H_1 k_{Mn(II)1} \Phi_{DO} 10^{2(pH1-7)} f_d \Phi_{Mn(II)1}^t \end{aligned}$$

Rearranging

$$\begin{aligned}
& \left( -\frac{H_1}{\Delta t} - w_{12} - w_2 \right) \Phi_{MnO_2 1}^{t+\Delta t} + w_{12} \Phi_{MnO_2 2}^{t+\Delta t} \\
& = -\frac{H_1}{\Delta t} \Phi_{MnO_2 1}^t - w_1 \Phi_{MnO_2 0} - H_1 k_{Mn(II) 1} \Phi_{DO} 10^{2(pH_1-7)} f_d \Phi_{Mn(II) 1}^t
\end{aligned}$$

And the finite difference scheme for layer 2

$$\begin{aligned}
H_2 \frac{\Phi_{MnO_2 2}^{t+\Delta t} - \Phi_{MnO_2 2}^t}{\Delta t} \\
= -w_{12} (\Phi_{MnO_2 2}^{t+\Delta t} - \Phi_{MnO_2 1}^{t+\Delta t}) + w_2 (\Phi_{MnO_2 1}^{t+\Delta t} - \Phi_{MnO_2 2}^{t+\Delta t}) - H_2 k_{MnO_2} \Phi_{MnO_2 2}^{t+\Delta t}
\end{aligned}$$

Rearranging

$$(w_{12} + w_2) \Phi_{MnO_2 1}^{t+\Delta t} + \left( -\frac{H_2}{\Delta t} - w_{12} - w_2 - H_2 k_{MnO_2} \right) \Phi_{MnO_2 2}^{t+\Delta t} = -\frac{H_2}{\Delta t} \Phi_{MnO_2 2}^t$$

## Model Testing

### Example Problem Set Up

The Version 3.6 OSPLM included a model example. This model was used in the testing of the new model algorithms. In addition, several examples were set-up to make sure the algorithms produced reasonable results. One of the best ways to check the model algorithms is to apply it to different model situations. One of these test cases is Wahiawa Reservoir, a reservoir in Oahu, Hawaii, USA. This example is shown in Appendix C.

### Sediment Oxygen Demand

Predicted sediment oxygen demand of the Oil Sands Pit Lakes Model (OSPLM) was compared with a simpler steady-state model (Ditoro, 2001) and a simple analytical model (Chapra, 1997). The predictions of the OSPLM using CE-QUAL-W2 version 3.6 were also calculated. Comparing model predictions to other models is helpful for determining the accuracy of the model. Sediment oxygen demand was predicted for varying BOD fluxes to the sediments (Figure 13). The simple analytical equation to predict SOD from Chapra (1997) is shown below:

$$SOD = \sqrt{2\kappa_D c_s J_{C^*}} \left\{ 1 - \operatorname{sech} \left[ \kappa_C \frac{o(0)}{SOD} \right] \right\} + r'_{on} a_{no} J_{C^*} \left\{ 1 - \operatorname{sech} \left[ \kappa_C \frac{o(0)}{SOD} \right] \right\}$$

where

- $r'_{on}$  = oxygen demand for nitrification, corrected for denitrification
- $o(0)$  = oxygen concentration in overlying water,  $g\ m^{-3}$
- $J_{C^*}$  = downward flux of organic carbon expressed as oxygen equivalents
- $c_s$  = methane saturation concentration,  $g\ m^{-3}$
- $\kappa_D$  = mass transfer coefficient for methane,  $m\ s^{-1}$
- $\kappa_C$  = mass transfer coefficient for oxygen,  $m\ s^{-1}$
- $a_{no}$  = nitrogen yield,  $gN\ gBOD^{-1}$

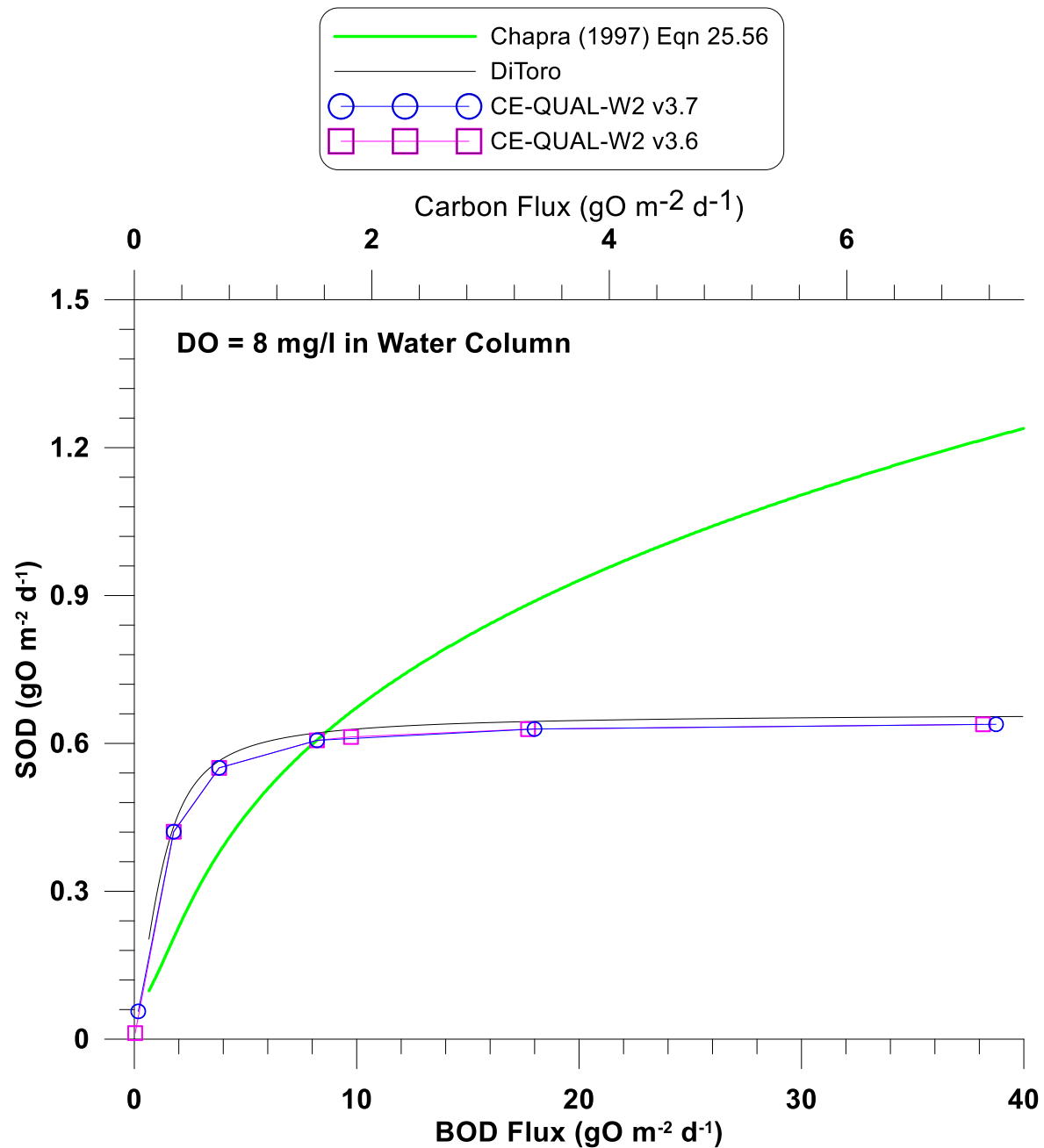


Figure 13. Sediment oxygen demand predictions for the CE-QUAL-W2 Oil Sands Pit Lakes Models versions 3.6 version 3.7 compared with the DiToro(2001) steady state model and a simple analytical solution provided by Chapra (1997).



## Summary

The Cumulative Environmental Management Association (CEMA) Oil Sands Pit Lake Model (OSPLM) was updated and enhanced. The original model (ERM and Golder Associates, 2013) was developed using the CE-QUAL-W2 Version 3.6 model of Cole and Wells (2008). The current code updates and enhancements included the following:

- (1) fixing coding issues noted in the original OSPLM (Wells ,2012)
- (2) updating the model to the latest release version of CE-QUAL-W2 Version 3.71 (Cole and Wells, 2013)
- (3) adding to the sediment model dynamic pH and temperature, metal complexation, phosphate fluxes, and dissolved oxygen consumption of resuspended organic matter
- (4) adding to the CE-QUAL-W2 model the release and transport from the sediments of methane and hydrogen sulfide

In addition the model was tested to evaluate whether the different model algorithms behaved as expected.

The model still needs to be calibrated to an Oil Sands pit lake in order to further test the algorithms in accordance with measured field data. The current testing of the model algorithms could be enhanced further by adding the following new algorithms:

1. Detailed mass balance checks on all sediment state variables: P, N, Fe, Mn, CH<sub>4</sub>, H<sub>2</sub>S, alkalinity, total inorganic carbon
2. Detailed sediment energy balances to check temperature predictions.
3. Additional comparisons of OSPLM predictions with simpler, analytical models. For instance, sediment resuspension predictions could be compared with analytical solutions.
4. Additional model testing by performing a full model calibration to a pit lake site.
5. Since this model will be applied in Canada, improvements in the CE-QUAL-W2 ice cover algorithm would improve the model predictive ability during ice cover conditions. Currently the model does not account for snow accumulation over the ice and has a steady-state ice cover algorithm that should be updated to a dynamic formulation.

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- Wells, S. A. (2012) Peer Review Comments on Oil Sands Pit Lake Model, Letter report to CEMA, February 12.

## Appendix A – Code issues identified in OSPLM

Wells (2012) identified several coding issues with the original OSPLM. These are shown in Table 3.

**Table 3. Peer review comments on the Oil Sands Pit Lake Model of ERM and Golder Associates (2013).**

Code subroutine or entry point	Comment
GasBubblesFormation	<pre>Henry(1) = HenryConst_H2S      !atm/M  H2S Henry(2) = HenryConst_CH4      !atm/M  CH4 Henry(3) = HenryConst_NH3      !atm/M  NH3 Henry(4) = HenryConst_CO2      !atm/M  CO2</pre> <ol style="list-style-type: none"> <li>1. The comment above needs to show the units as L atm/mol rather than atm/M (see earlier comment by Wells for the report).</li> <li>2. Also, since this piece of code (and the next 10 or so lines) are called for each segment for each time update, perhaps these static constants can be moved to a module to improve computational efficiency.</li> </ol>
GasBubblesFormation	<pre>P0      = 9800      !N/m² Mw(1)   = 36        !H2S  gm/mol Mw(2)   = 16        !CH4  gm/mol Mw(3)   = 17        !NH3  gm/mol Mw(4)   = 44        !CO2  gm/mol</pre> <p>Add decimal points for real numbers for good coding practice. There are many cases in the code where this is a practice. I will only show places where this causes issues in subsequent comments.</p>
GasBubblesFormation	<pre>Pcrit 1.32*(CritStressIF**6/(YoungModulus*Nbubbles*Vbub))**0.2 + P0 =</pre> <p>Very minor, but could use 1.324 rather than 1.32 in the constant above.</p>
GasBubblesFormation	<pre>SourceT = SourceT + Source !Ctot(nGas) = Ctot(nGas) + Source*DeltaT C0B(nGas) = Ctot(nGas)/(1+K(nGas))</pre> <p>The source term for gas production was commented out. Hence, the procedure as documented in the report on p. 25 and p. 26 (Equation 36) is not being followed. This seems like an inadvertent commenting out of the code for testing purposes.</p>
GasBubblesFormation	<pre>DiffVolume = DiffVolume*BubbRelScale</pre> <p>The variable BubbRelScale is an input to the model but is not documented in the main text of the report. Provide documentation.</p>

Code subroutine or entry point	Comment
GasBubblesFormation	<pre> If(UseReleaseFraction)Then     Vbubbles =     CritStressIF**6/(YoungModulus*((Pcrit*CrackCloseFraction)/1.32 )**5)     DiffVolume = BubbRelFraction*(Vbub*Nbubbles - Vbubbles) End If </pre> <p>The variable UseReleaseFraction is an input to the model but is not documented in the main text of the report. This switches to a slow release of the bubbles and needs to be documented in the write up.</p>
GasBubblesFormation	<pre> If(PbubbT &gt; Pcrit .and. .NOT. CrackOpen(SegNumI))Then     CrackOpen(SegNumI) = .TRUE.     Vbubbles = CritStressIF**6/(YoungModulus*((PbubbT- P0)/1.32)**5)     DiffVolume = Vbub*Nbubbles - Vbubbles     DiffVolume = DiffVolume*BubbRelScale     If(UseReleaseFraction)Then         Vbubbles =         CritStressIF**6/(YoungModulus*((Pcrit*CrackCloseFraction)/1.32 )**5)         DiffVolume = BubbRelFraction*(Vbub*Nbubbles - Vbubbles)     End If     LastDiffVolume(SegNumI) = DiffVolume     NbubbLost = (DiffVolume)/Vbub     NbubblesP = Nbubbles     Nbubbles = Nbubbles - NbubbLost     Do nGas = 1, NumGas         CgB(nGas) = CgB(nGas)*(Vbub*NbubblesP - DiffVolume)/(Vbub*NbubblesP)         C0B(nGas) = CgB(nGas)/K(nGas)         Ctot(nGas) = C0B(nGas)*(1+K(nGas))     End Do !nGas End If If(CrackOpen(SegNumI))Then     NbubblesP = Nbubbles     Nbubbles = Nbubbles - NbubbLost </pre> <p>When the first condition is correct and then CrackOpen is set to TRUE, during the next IF test, Nbubbles is again subtracted from NbubbLost. It appears that Nbubbles is inadvertently subtracted twice by NbubbLost.</p>
GasBubblesFormation	<pre> Do nRelArr = 1, NumBubRelArr </pre> <p>Variable NumBubRelArr is an input variable set to 2000. It is not clear from the documentation what this represents. Add documentation in the report for what the value of NumBubRelArr represents and why 2000 was chosen as an input.</p>

Code subroutine or entry point	Comment
CEMABubblesRiseVelocity	$W = \text{dlog}_{10}(N_D)$ <p>In the report on p. 28 in Table 2, change <math>W = \log N_D</math> to <math>W = \log_{10} N_D</math> for clarity.</p>
CEMABubblesRiseVelocity	$\text{Reynolds} = N_D/24 - 1.7569d-4*N_D^{**2} + 6.9252d-7*N_D^{**3} - 2.3027d-10*N_D^{**4}$ <p>Should add decimal point to <math>N_D/24</math> so that it is <math>N_D/24.</math> To avoid potential issues with mixed mode arithmetic. Throughout this section there are many cases where decimal points should be added for good modeling practice.</p>
CEMABubblesRiseVelocity	$H = (4/3)*E_o*M^{**(-0.149)}*(\text{DynVisc}/\text{DynVisc})^{**(-0.14)}$ <p>This is a coding error since <math>4/3=1</math> rather than the expected <math>4./3.=1.33</math>. Add decimal points. This line occurs twice in the subroutine.</p>
CEMABubblesRiseVelocity	<pre> If(H &lt; 59.3)Then   J = 0.94*H**0.757 Else   J = 3.42*H**0.441 End If </pre> <p>Make a note in the report on p. 28 that J is described when <math>H &lt; 59.3</math> and <math>&gt; 59.3</math>. In the report it says that J is defines as <math>0.94H^{0.757}</math> when <math>2 &lt; H &lt; 59.3</math>.</p>
CEMABubbWatTransfer	<pre> Henry(1) = HenryConst_H2S      !atm/M  H2S Henry(2) = HenryConst_CH4      !atm/M  CH4 Henry(3) = HenryConst_NH3      !atm/M  NH3 Henry(4) = HenryConst_CO2      !atm/M  CO2 BubSedT  = 273.15 + CEMAPWTemperature !K Mw(1)    = 36                  !H2S  gm/mol Mw(2)    = 16                  !CH4  gm/mol Mw(3)    = 17                  !NH3  gm/mol Mw(4)    = 44                  !CO2  gm/mol </pre> <p>This code is repeated here as in the subroutine GasBubbleFormation. One could put these in a module that does not need resetting the static values each time the subroutine is called.</p>

Code subroutine or entry point	Comment
CEMABubbWatTransfer	<pre> Do nGas = 1, NumGas BubblNumber = BubblesLNumber(SegNumI, nRelArr) KValue(1) = Henry(1)/GasConst_R/(T1(BubblNumber,SegNumI) + 273.15) KValue(2) = Henry(2)/GasConst_R/(T1(BubblNumber,SegNumI) + 273.15) KValue(3) = Henry(3)/GasConst_R/(T1(BubblNumber,SegNumI) + 273.15) KValue(4) = Henry(4)/GasConst_R/(T1(BubblNumber,SegNumI) + 273.15)  Change this for code efficiency to  Do nGas = 1, NumGas BubblNumber = BubblesLNumber(SegNumI, nRelArr) KValue(nGas) = Henry(nGas)/GasConst_R/(T1(BubblNumber,SegNumI) + 273.15) </pre>
CEMABubbWatTransfer	<pre> BubbDissSrcSnk = BubbWatGasExchRate*(EqbDissConcentration - C1(BubblNumber,SegNumI,1+nGas))    !g/m³/s </pre> <p>This comment appears a few times in this review. The synchronizing of the CE-QUAL-W2 variables with the new code may need some more thought. It appears that the last subscript in the C1 array, 'nGas+1', is dependent on having the same number of active constituents as in the example problem. If the model user turned on TDS or added additional generic constituents, for example, this subscript would be incorrect and all further calculations would be in error. Hence, I would recommend making the subscript order more robust in translating from the CE-QUAL-W2 state variables to the new variables in the CEMA code.</p>
CEMABubblesTurbulence	<pre> If(k == KB(SegNumI))Then AZ(K,SegNumI) = AZ(K,SegNumI) !+ BottomTurbulence(SegNumI) Else AZ(K,SegNumI) = AZ(K,SegNumI) !+ TempBubbDiam/TempRelVelocity End If </pre> <p>Why are the terms in green not implemented in the code? Hence, there is no influence on bubbles for enhanced vertical mixing in the CE-QUAL-W2 model. Also, in the report on p. 27 Equation 41, the correct form is used: <math>v_b = d_b \times V_R</math>. Above in the commented text it is incorrect incorrect – it should be</p> <p>TempBubbDiam*TempRelVelocity</p>

Code subroutine or entry point	Comment
CEMAComputeTurbidity	<pre> Do K = KT, KB(SegNumI) CellTSSValue = C1(K,SegNumI,6) C1(K,SegNumI,6)=exp(CoeffA_Turb*log(CellTSSValue) + CoeffB_Turb) C2(K,SegNumI,6)=exp(CoeffA_Turb*log(CellTSSValue) + CoeffB_Turb) </pre> <p>The value of turbidity is hard-wired to concentration #6 in the CEQUAL-W2 code. This presents a problem if other model users add TDS or other generic constituents to the model. I would recommend setting turbidity as a derived variable.</p>
CEMASedimentDiagenesis	<pre> Common /CEMASedFlxVarsBlk/iTemp, RegnNum, iter, InitConRegn, &amp; SD_POC_L_Fr, SD_POC_R_Fr, </pre> <p>Suggest if possible to eliminate Common blocks and put variables in Modules for coding consistency.</p>
CEMASedimentDiagenesis	<pre> MFTSedFlxVars(SegNumI,5) = SDRegnH2S_T(InitConRegn) MFTSedFlxVars(SegNumI,6) = SDRegnH2S_T(InitConRegn) MFTSedFlxVars(SegNumI,14) = SDRegnNH3_T(InitConRegn) MFTSedFlxVars(SegNumI,15) = SDRegnNH3_T(InitConRegn) </pre> <p>The subscripts are incorrect for the highlighted code. This is the danger of using fixed numbers rather than a variable for the index. #5 and #6 should be for NH3, not H2S, and #14 and #15 should be for H2S. This is based on definitions under</p> <p>Entry WriteCEMASedimentFluxVariables where</p> <pre> SD_NH3p2(2) = MFTSedFlxVars(SegNumI,4) SD_NH3Tp2(1) = MFTSedFlxVars(SegNumI,5) SD_HSTp2(1) = MFTSedFlxVars(SegNumI,14) SD_HSTp2(2) = MFTSedFlxVars(SegNumI,15) </pre>
CEMASedimentDiagenesis	<pre> SD_CH40 = MAX(C1(KB(SegNumI),SegNumI,3),0.0) !Generic constituent 2 </pre> <p>As mentioned before, the use of static indexes, such as '3' above, can lead to unexpected problems if the model user has a different number of generic constituents or also models TDS/salinity.</p>
ComputeGenBODFate	<pre> !Only if there are aerobic conditions If(SD_O20 &gt; 1.0e-10)SD_BOD = SD_s * (SedGenBODConc(GenBODNum,SegNumI,1) SedGenBODConc0(GenBODNum)) </pre> <p>For code consistency, use 'SD_Ox_Threshol' rather than '1.0E-10'.</p>
ComputeCEMADiagenesisSourceSinks	Empty subroutine even though called from main program.

Code subroutine or entry point	Comment
CEMASedimentModel	<pre> Do k = kt, KB(SegNumI)   CEMASedConc(SegNumI, K) = C1(K, SegNumI, NSSS) End Do !k </pre> <p>The suspended sediment only uses the first suspended solids group identified by NSSS. If the model user has multiple suspended sediment size fractions between NSSS and NSSE, all of these inorganic SS groups should be accounted for. Another issue, should the organic suspended solids also be accounted for here? It might be better to use the derived variable for Total suspended solids unless one wants to parse out the scour/deposition of each group of suspended solids.</p>
CEMASedimentModel	<pre> CEMACumPWRelease(SegNumI) = CEMACumPWRelease(SegNumI) + TotalPoreWatRemoved !m³ </pre> <p>Are there other pore water release mechanisms other than TotalPoreWatRemoved? It is unclear why this is additive as if there were other mechanisms.</p>
CEMASedimentModel	<pre> BedPorosity(SegNumI) = 1.d0 - VolumeofSedimentBed1/VolumeofSedimentBed2*(1- BedPorosity(SegNumI)) VolumeofPorewater2 = VolumeofSedimentBed2*BedPorosity(SegNumI) TotalPoreWatRemoved = VolumeofPorewater1 - VolumeofPorewater2 PorewaterRelRate(SegNumI) = TotalPoreWatRemoved/dlt !m³/s CEMACumPWRelease(SegNumI) = CEMACumPWRelease(SegNumI) + TotalPoreWatRemoved !m³ CEMACumPWReleaseRate(SegNumI) = CEMACumPWRelease(SegNumI)/dlt !m³/s  If(BedPorosity(SegNumI) &lt; 0.d00)Then   TotalPoreWatRemoved = 0.d00   BedPorosity(SegNumI) = 0.d00   EndBedConsolidation(SegNumI) = .TRUE. </pre> <p>Since the bed porosity cannot be less than 0, it is possible that the CEMACumPWRelease is overestimated when BedPorosity=0 since CEMACumPWRelease is defined before TotalPoreWatRemoved is set to zero. I would suggest the following: (1) Compute BedPorosity; (2) If BedPorosity is less than 0, then set it to 0 and recalculate bed consolidation; (3) then TotalPoreWatRemoved and CEMACumPWRelease would be OK.</p>



Code subroutine or entry point	Comment
CEMASedimentModel	<pre> Do k = kt, KB(SegNumI) C1(K,SegNumI,NSSS) = CEMASedConc(SegNumI, K) End Do !k </pre> <p>Similar issue as raised above. What if the user has 4 inorganic suspended solids groups with different settling velocities. This code only accounts for the first one.</p>
CEMASedimentProcesses	<pre> !Calculate settling   If(IncludeFFTLayer .and. FFTActive)Then     SSettle = FFTLayerSettVel*CEMASedConc(SegNumI, KB(SegNumI))   End If   If(IncludeFFTLayer .and. .NOT. FFTActive)Then     SSettle = 0.d00   End If   If(.NOT. IncludeFFTLayer)Then     SSettle = CEMASedimentSVelocity*CEMASedConc(SegNumI, KB(SegNumI))   End If !Net Flux   SNetFlx = SScour - SSettle !gm/m2/s </pre> <p>A similar question as raised above. The SSettle, the flux of suspended solids to the sediment layer, only includes the first suspended solids group and no organic material. Should this be generalized to include organics and other suspended solids groups?</p>
CEMACalculateScour	<p>Dks = CEMAParticleSize</p> <p>Sediment scour is based only on one particle size in the bed. If multiple suspended solids groups are considered as settling to the bed, then perhaps the bed needs also to have multiple size fractions?</p>
CEMACalculateScour	<pre> !Limit bottom velocity           VelTemp = Min(VelTemp,0.01)           VelTemp = sqrt(G)*VelTemp/FRIC(SegNumI) !#####CHECK </pre> <p>The friction factor, FRIC, can be either a Mannings or Chezy coefficient. The above calculation needs to be revised to account for either friction type.</p>
CEMACalculateScour	<pre> VelTemp = 0.5*(u(K,SegNumI) + u(K,SegNumI-1)) VelTemp = dsqrt(VelTemp**2) </pre> <p>It is not clear why the square root of a squared variable is taken. It would be computationally less expensive just to take the absolute value of VelTemp.</p>

Code subroutine or entry point	Comment
CEMAUpdateVerticalLayering	<pre> VolumeIncreased = VolumeNew - VolumePresent !Calculate surface area SurfaceAreaWB = 0.d00 Do JW=1, NWB   KT = KTWB(JW)   Do JB=BS(JW), BE(JW)     IU = CUS(JB)     ID = DS(JB)     Do SegNumI = IU, ID       SurfaceAreaWB = SurfaceAreaWB + B(KT,SegNumI)*DLX(SegNumI)     End Do !SegNumI   End Do !JB End Do !JW SEChange = VolumeIncreased/SurfaceAreaWB </pre> <p>The bed elevation is changed by 2 processes: (1) bed consolidation and (2) scour/deposition of solids. This is computed in another routine as</p> $\text{BedElevationLayer}(\text{SegNumI}) = \text{BedElevationLayer}(\text{SegNumI}) - \text{BedConsolidRate}(\text{SegNumI}) * \text{dlt}$ <p>and</p> $\text{BedElevationLayer}(\text{SegNumI}) = \text{BedElevationLayer}(\text{SegNumI}) - \text{SNetFlx} * \text{dlt} / (\text{CEMASedimentDensity} * 1000.d0)$ <p>The SNetFlx term is defined as</p> $\text{SNetFlx} = \text{SScour} - \text{SSettle}$ <p>It is clear that bed consolidation affects the water surface elevation, but scour/deposition should not affect the surface elevation. Hence, one should separate the bed consolidation from scour/deposition terms in computing the water surface elevation correction.</p>

Code subroutine or entry point	Comment
DoCEMAMFTSedimentDiagen	<pre> SD1_Ammonia = SD_NH3(1)/(1 + 10**(-SD_pHValue(SegNumI))/10**(- NH4_NH3_Eqb_Const)) SD1_Ammonium = SD_NH3(1) - SD1_Ammonia SD2_Ammonia = SD_NH3(2)/(1 + 10**(-SD_pHValue(SegNumI))/10**(- NH4_NH3_Eqb_Const)) SD2_Ammonium = SD_NH3(2) - SD2_Ammonia !Calculate dissolved &lt;--&gt; gaseous phase distribution SedTemp = SD_Tw + 273.15 </pre> <p>The value of NH4_NH3_Eqb_Const is given as a constant and is not temperature dependent. Since this is very sensitive to temperature, it would be easy to add temperature dependency since SD_Tw is available in the model. Currently temperature is constant, but adding this dependency would allow for the code to be more flexible in the future.</p> <p>For example the temperature dependency of this coefficient is based on the equilibrium coefficient K where K is defined as</p> $K = \frac{\{NH_3\}\{H^+\}}{\{NH_4^+\}} = \frac{\gamma_{NH3} \gamma_H}{\gamma_{NH4}} \frac{[NH_3][H^+]}{[NH_4^+]}$ <p>The relationship between K and temperature is</p> $K = 10^{(-0.09018 - \frac{2729.92}{T+273.15})}$ <p>where T is the temperature in degrees C and K is in units of moles/liter (National Research Council, 1979).</p>
Comment, p. 11/21 in Appendix A of the report	<p>The values of the nitrification rates in the aerobic layer SRegAe_NH3_NO3_L and SRegAe_NH3_NO3_H are set to the same values of 0.131 m/d. Should not these values be different above and below the DO threshold? Similar question for the denitrification rate.</p>
Comment, p. 8 Figure 3 in the Report #09-1336-1008	<p>The new state variables in the water column, such as CH4 and H2S, do not appear to have any sources/sinks other than dissolution into bubbles and oxidation according to Figure 3 in the report. These state variables need also to have a reaeration component, such as</p>

Code subroutine or entry point	Comment
	<div data-bbox="618 254 1174 531" data-label="Diagram"> </div> <p data-bbox="592 552 1382 583">Then the source sink term for reaeration would be something like:</p> $S = \underbrace{A_{sur} K_L}_{\text{reaeration}} (-\Phi)$ <p data-bbox="959 810 1047 842">where:</p> <p data-bbox="630 842 1247 877"><math>A_{sur}</math> = surface area of surface computational cell, <math>m^2</math></p> <p data-bbox="646 877 1096 913"><math>K_L</math> = interfacial exchange rate, <math>m \text{ sec}^{-1}</math></p> <p data-bbox="654 913 1242 949"><math>\Phi</math> = constituent concentration (<math>H_2S</math> or <math>CH_4</math>), <math>g \text{ m}^{-3}</math></p> <p data-bbox="592 997 1419 1029">The reaeration rate can be determined using the penetration theory</p> $K_a = 2\sqrt{\frac{Df}{\pi}} \frac{1}{h}$ <p data-bbox="592 1098 1419 1354">for gas transfer, i.e., where <math>f</math> is the turbulence frequency of surface renewal, <math>D</math> is the molecular diffusion coefficient for <math>O_2</math> and <math>h</math> is the depth, once the reaeration coefficient for dissolved oxygen is determined, then the value of the reaeration coefficient <math>k_{H_2S}</math> for <math>H_2S</math> is determined from the following equation (Thibodeaux, 1996):</p> $k_{H_2S} = k_{O_2} \sqrt{\frac{D_{H_2S}}{D_{O_2}}}$ <p data-bbox="592 1556 662 1587">Using</p> $\frac{D_A}{D_B} = \sqrt{\frac{MW_B}{MW_A}}$ <p data-bbox="592 1707 1419 1780">where <math>MW</math> is the molecular weight of the component</p> <p data-bbox="592 1833 651 1864">then</p>

Code subroutine or entry point	Comment
	$k_{H_2S} = k_{O_2} \left( \frac{MW_{O_2}}{MW_{H_2S}} \right)^{0.25}$ <p>Given the molecular weights of oxygen and hydrogen sulfide :</p> $MW_{O_2} = 32.00 \text{ g/mol}$ $MW_{H_2S} = 34.08 \text{ g/mol}$ <p>the reaeration coefficient for hydrogen sulfide is:</p> $k_{H_2S} = k_{O_2} \left( \frac{MW_{O_2}}{MW_{H_2S}} \right)^{0.25} = k_{O_2} \times 0.984$ <p>Likewise for methane</p> $MW_{CH_4} = 16.04 \text{ g/mol}$ <p>The reaeration coefficient <math>k_{CH_4}</math> is:</p> $k_{CH_4} = k_{O_2} \left( \frac{MW_{O_2}}{MW_{CH_4}} \right)^{0.25} = k_{O_2} \times 1.188$

## Appendix B – Updated Model User Updates

The new OSPLM in CE-QUAL-W2 Version 3.7 includes a new input file as for the original OSPLM model in Version 3.6.

### Model files

The model files include new FORTRAN90 subroutines for compiling into the model as well as updated output files for the model. New FORTRAN90 source codes files specific to the OSPLM are listed below:

- CEMA Bubbles Code 01.f90
- CEMA FFT Layer 01.f90
- CEMA Input 01.f90
- CEMA Input Files Read 01.f90
- CEMA Output 01.f90
- CEMA Sediment Flux Model 03.f90
- CEMA Sediment Model 03.f90
- CEMA Turbidity 01.f90

New input files are listed in Table 4.

**Table 4. New input files used on the OSPLM.**

File Name	Description
W2_CEMA_Input.npt	setup for the all the CEMA related inputs except for those of the enhanced pH buffering and non-conservative alkalinity subroutines
pH_buffering.npt	Inputs for enhanced pH buffering and non-conservative alkalinity subroutines
User specified bed consolidation rate file(s)	Time series file of bed consolidation rate

### How to run the model

#### Compiling the model

The list of model FORTRAN source code files is shown in Table 5. We used the Intel Visual FORTRAN 13 compiler to develop an executable. The FORTRAN compiler used to develop an executable and make these test runs was Intel Visual FORTRAN V13.0 setup as a Windows application using the following options:

```
/nologo /O2 /warn:interfaces /real_size:64 /fp:source /module:"x64\Release\\" /object:"x64\Release\\" /Fd"x64\Release\vc110.pdb" /libs:static /threads /winapp /c
```

For the “CEMA Sediment Model 03.f90” and “CEMA Sediment Flux Model 03.f90” source files:

```
/nologo /O2 /recursive /warn:nointerfaces /real_size:64 /fp:source /module:"x64\Release\\" /object:"x64\Release\\" /Fd"x64\Release\vc110.pdb" /libs:static /threads /winapp /c
```

*If using a different FORTRAN compiler, always set the default REAL kind to double precision.*

A User's Forum has been set up on the web where support from the developers and other users can be obtained. The forum is located at <http://w2forum.cee.pdx.edu>

**Table 5. CE-QUAL-W2 source code files.**

















Source Filename
aerate.f90
az.f90
balances.F90
CEMA Bubbles Code 01.f90
CEMA FFT Layer 01.f90
CEMA Input 01.f90
CEMA Input Files Read 01.f90
CEMA Output 01.f90
CEMA Sediment Flux Model 03.f90
CEMA Sediment Model 03.f90
CEMA Turbidity 01.f90
date.f90
density.f90
endsimulation_PAR.F90
envir_perf.f90
fishhabitat.f90
gas-transfer.f90
gate-spill-pipe.f90
heat-exchange.f90
hydroinout.F90
init-cond.F90
init-geom.F90
init-u-elws.f90
init.F90
input_par.F90
layeraddsub.F90
macrophyte-aux.f90
output.f90
outputa2w2tools.F90

Source Filename
outputinitw2tools.F90
restart.f90
screen_output_intel.f90
shading.f90
tdg.f90
temperature_PAR.F90
time-varying-data.f90
transport_PAR.f90
update.F90
w2modules_par.F90
w2_37_win.f90
water-quality.f90
waterbody.f90
withdrawal.f90
wqconstituents_par.F90

### Running the model

The OSPLM will typical consist of a list of files in a single directory:



Name	Date modified	Item type	Size
 preW2-37_64.exe	7/2/2013 3:20 PM	Application	5,322 KB
 w2_ivf64.exe	9/18/2013 3:31 PM	Application	4,085 KB
 BML_bth.npt	9/24/2013 11:11...	NPT File	1 KB
 cin_br1.npt	12/10/2013 3:01...	NPT File	1 KB
 graph.npt	1/6/2014 3:32 PM	NPT File	8 KB
 met.npt	9/24/2013 11:11...	NPT File	1 KB
 pH_buffering.npt	10/25/2013 11:2...	NPT File	1 KB
 qin_br1.npt	1/7/2014 9:53 AM	NPT File	1 KB
 qot_br1.npt	6/22/2009 5:50 PM	NPT File	7 KB
 Regn1.npt	8/9/2010 12:29 PM	NPT File	7 KB
 Regn2.npt	2/2/2010 5:15 PM	NPT File	7 KB
 shade.npt	9/24/2013 10:43...	NPT File	1 KB
 tin_br1.npt	12/10/2013 11:4...	NPT File	1 KB
 W2_CEMA_Input.npt	1/26/2014 1:38 PM	NPT File	10 KB
 w2_con.npt	1/26/2014 1:36 PM	NPT File	27 KB
 wsc.npt	9/24/2013 10:43...	NPT File	1 KB

**Figure 14. Example file set for OSPLM.**

Steps required to set-up the CE-QUAL-W2 model on your PC are shown below:

1. Copy model input files and executables into a single directory on your computer
2. Install the W2 GUI and post-processor– this program is useful for editing the control file (**w2\_con.npt**), evaluating the model grid after it has already been constructed, and post-processing model results.
3. Assemble input files as well as w2 codes for the model executable (**w2\_ivf64.exe**) and preprocessor (**preW2-37\_64.exe**) on your hard disk

**Typical questions:**

**Can you run CE-QUAL-W2 on a UNIX/LINUX or other platform?** Yes. But you will need to recompile and tweak the source code- not trivial.

**What is the difference between the 32 and 64 bit versions?** These are windows executables and will run on Windows XP, Vista, 7, and 8. The 32 bit executables will run on both 32 and 64 bit windows operating systems (OS). The 64 bit will only run on the 64 bit versions of the windows OS. Generally we have found that the 64 bit executes faster (up to 10%) than the 32 bit on a 64 bit OS.

Note that the CE-QUAL-W2 model reads in ASCII text files as input files. Output files are also generally ASCII text files for post-processing and evaluation.

To set up and run a OSPLM the following steps are required:

1. **Construct all boundary condition files** – flow rates, temperatures, and concentrations for all inflows, meteorological conditions for each waterbody, water levels for head BCs, shading for each segment, wind sheltering file for segments as a f(time)

Look in the directory and notice all the files with the ‘npt’ extension. These are input files that the user must construct. Examine several of the files: the meteorological file (**met.npt**) and a flow file (**Qin\_br1.npt**) by opening a text editor like NOTEPAD to look at the file structure. We prefer to use the program Notepad++, which is a free text editor that is much more powerful than Notepad. Google NOTEPAD++ for installation instructions/location.

2. **Develop the Model Grid** – this involves developing a bathymetry file for each water body. Use a text editor to open the existing bathymetry file for Example 1 (**BML\_bth.npt**). Now open the GUI Interface (do this by using the file **W2Control37.exe**) and click on CON for the control file and BTH for the bathymetry editor. You can view the bathymetry graphically with views of the side, top and end of the segments by clicking on appropriate buttons.

Note that the model also now uses “csv” file format so that the grid can be viewed and edited directly in Excel rather than the more cumbersome bathymetry file format as shown below in a file named **bth.csv**.

S1981 Bluestone Reservoir Bathymetry																																				
SEG 1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32				
DLX	1046.4	1046.4	1046.4	965.9	965.9	764.7	764.7	1046.4	1046.4	1073.2	1073.2	1073.2	1126.9	1126.9	1180.5	1180.5	1180.5	912.2	912.2	912.2	804.9	804.9	804.9	804.9	804.9	858.5	858.5	858.5	1006.1	1006.1	457.3	457.3				
ELWS	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1	430.1				
PHFO	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142	3.142					
FRCT	70	70	70	70	70	70	70	70	70	70	70	70	70	70	70	70	70	70	70	70	70	70	70	70	70	70	70	70	70	70	70	70				
LAYERH	BR1																																			
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
0.5	0	335	335	335	335	364	364	362	362	327	327	327	423	423	438	438	438	472	472	472	490	490	457	457	457	501	501	501	516	516	487	487				
0.5	0	231	231	231	231	254	254	255	255	312	312	312	406	406	426	426	426	466	466	466	486	486	453	453	453	498	498	498	509	509	483	483				
0.5	0	228	228	228	228	243	243	248	248	298	298	298	388	388	413	413	413	460	460	460	482	482	449	449	449	494	494	494	502	502	480	480				
0.5	0	224	224	224	224	231	231	241	241	285	285	285	370	370	400	400	400	453	453	453	477	477	444	444	444	491	491	491	495	495	476	476				
0.5	0	220	220	220	220	219	219	233	233	272	272	272	351	351	387	387	387	446	446	446	472	472	440	440	440	487	487	487	488	488	473	473				
0.5	0	215	215	215	215	206	206	225	225	259	259	259	332	332	373	373	373	439	439	439	467	467	435	435	435	484	484	484	481	481	467	467				
0.5	0	202	202	202	202	188	188	208	208	247	247	247	324	324	359	359	359	431	431	431	462	462	430	430	430	480	480	480	473	473	465	465				
0.5	0	192	192	192	192	161	161	199	199	234	234	234	291	291	345	345	345	422	422	422	457	457	425	425	425	476	476	476	465	465	461	461				
0.5	0	173	173	173	142	142	189	189	222	222	222	222	269	269	330	330	330	414	414	414	451	451	420	420	420	472	472	472	458	458	457	457				
0.5	0	0	0	0	130	130	130	178	178	208	208	247	247	315	315	315	315	404	404	404	445	445	415	415	415	468	468	468	450	450	453	453				
0.5	0	0	0	0	125	125	125	166	166	195	195	195	223	223	288	288	288	395	395	395	440	440	409	409	409	465	465	465	442	442	449	449				
0.5	0	0	0	0	120	120	153	153	181	181	181	199	199	282	282	282	384	384	384	433	433	404	404	404	460	460	460	434	434	445	445	0				
0.5	0	0	0	0	110	139	139	167	167	167	173	173	265	265	265	372	372	372	427	427	397	397	397	397	456	456	456	426	426	440	440	0				
0.5	0	0	0	0	135	135	151	151	151	151	145	145	246	246	246	360	360	360	419	419	391	391	391	391	451	451	451	417	417	436	436	0				
0.5	0	0	0	0	0	0	0	0	0	0	130	134	134	134	116	116	227	227	227	346	346	346	412	412	384	384	384	447	447	408	408	431	0			
0.5	0	0	0	0	0	0	0	0	0	0	0	114	114	114	100	100	209	209	209	330	330	330	404	404	377	377	442	442	400	400	426	0				
0.5	0	0	0	0	0	0	0	0	0	0	0	40	100	90	100	184	184	184	311	311	311	396	396	369	369	369	436	436	391	391	422	0				
0.5	0	0	0	0	0	0	0	0	0	0	0	40	80	90	160	160	160	288	288	288	386	386	361	361	361	431	431	381	381	411	411	0				
0.5	0	0	0	0	0	0	0	0	0	0	0	0	40	80	134	134	134	258	258	258	376	376	352	352	352	426	426	372	372	411	411	0				
0.5	0	0	0	0	0	0	0	0	0	0	0	0	75	104	104	104	215	215	215	364	364	342	342	342	420	420	420	362	362	406	406	0				
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	100	100	90	146	146	146	351	351	330	330	330	413	413	413	352	352	401	401	0				
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	90	80	83	83	334	334	334	317	317	317	407	407	407	342	342	394	394	0					
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	44	44	44	313	313	302	302	302	400	400	400	331	331	388	0				
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	30	40	279	279	282	282	282	392	392	392	320	320	382	382	0				
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	30	68	68	251	251	251	384	384	308	308	375	375	0			
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	39	39	72	72	72	375	375	375	297	297	368	368	0			
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	30	34	34	54	365	365	365	284	284	360	360	0				
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	30	30	40	353	353	353	271	271	352	352	0					
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	340	340	257	257	344			
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	322	322	243	243	344			
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	296	296	226	226	324			
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100	134	210	210	312			
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	130	130	191	191	299			
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	50	50	171	171	285			
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	30	147	147	266	266			
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	117	117	241	241	0		
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	75	75	197	197	0		
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	57	57	50	50	0	
0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		

3. **Edit the Control File** – this file, **w2\_con.npt**, is the central file for describing how the model will run. This file tells the code when the model starts, ends, where the inflows/outflows are located, names of files, kinetic parameters for the water column, and items you cannot even imagine. Open this file in a text editor or open it using the GUI **W2Control37.exe**
<

5. **Run the Preprocessor** – this file, **preW2-37\_64.exe**, checks for model errors in the control file, bathymetry file, and all boundary condition files. Double click on the executable and look at the preprocessor screen. This file writes out between 1 and 3 files: **pre.opt** (an echo of input data and other useful items), **pre.err** (if fatal errors), and **pre.wrn** (if warnings). Make sure you look at **pre.wrn** and **pre.err** files.
6. **Run the W2 Model** – the file **w2\_ivf64.exe** is the W2 model code. Double click on the w2 executable and notice the dialog box and the dynamic animation boxes for the simulation.
7. **Evaluate OUTPUT files or Model Results** – W2 outputs files have an extension 'opt'. Open the file **snp1.opt** (a snapshot file) using NOTEPAD. There are other files you can use with Excel for easy plotting, such as TSR files and Spreadsheet files. At the workshop we will be using Tecplot360 from [www.tecplot.com](http://www.tecplot.com) for animating the results as well as the w2tools post-processor.

## OSPLM input files

In addition to the normal CE-QUAL-W2 input files, the OSPLM model reads the input files 'W2\_CEMA\_Input.npt', 'pH\_buffering.npt' and possibly bed consolidation rate input files (file name specified by user). The 'W2\_CEMA\_Input.npt' contains the setup for the all the CEMA related inputs except for those of the enhanced pH buffering and non-conservative alkalinity subroutines. The enhanced pH buffering inputs are read from 'pH\_buffering.npt'. Enhanced pH buffering and non-conservative alkalinity are turned on using additional switches added to the control file card MISCELL.

Inputs for the 'W2\_CEMA\_Input.npt' input file are described below following the sample input file. The descriptions have been adapted and expanded from those in ERM and Golder Associates (2011).

### W2\_CEMA\_Input.npt Sample Input file:

```
$Additional CEMA related W2 input
$Please see help file for input description
$All lines starting with $ are comments and disregarded by the model
"H2S Constituent Number (Generic Constituent)", 2
"CH4 Constituent Number (Generic Constituent)", 3
"SO4 Constituent Number (Generic Constituent)", 4
"Turbidity Constituent Number (Generic Constituent)", 6
"Fe(II) Constituent Number (Generic Constituent)", 7
"FeOOH Constituent Number (Generic Constituent)", 8
"Mn(II) Constituent Number (Generic Constituent)", 9
"MnO2 Constituent Number (Generic Constituent)", 10
"Mature Fine Tailing (MFT) Constituent Number (ISS Constituent)", 11
"Switch to perform bed consolidation", .FALSE.
"Fraction of layer thickness at which water layer is added", 1.0
"Number of bed consolidation regions", 1
"Starting segment for regions", 2
"Ending segment for regions", 4
```

"Data type for bed consolidation for each region (0: Constant, 1: Time  
 varying),", 1  
 "Bed consolidation rate (m/d),", 0.02739726  
 "Bed consolidation data file,", "Regn1.npt,"  
 "Initial bed elevation in meters,", 0.1  
 "Initial sediment bed porosity,", 0.8  
 "Maximum Water Surface Elevation,", 10.0  
 "Porewater Temperature (C),", 20.0  
 "Porewater pH,", 8.5  
 "Sediment bed particle size in microns,", 100  
 "Sediment type 1: Cohesive, 2: Non-cohesive,", 2  
 "Sediment bulk density (kg/m<sup>3</sup>),", 2600  
 "Sediment particle settling velocity (m/d),", 5.0  
 "Include sediment resuspension and deposition processes,", .TRUE.  
 "Write bed elevation snapshot output,", .TRUE.  
 "Write bed porosity snapshot output,", .TRUE.  
 "Include FFT Layer,", .FALSE.  
 "FFT Layer Number of Periods,", 5  
 "FFT Layer Start Times,", 1,65,125,200,300  
 "FFT Layer End Times,", 50,100,175,250,400  
 "Initial tailings concentration in FFT (gm/m<sup>3</sup>),", 360000  
 "Settling velocity of FFT to MFT (m/d),", 0.d0  
 "Move FFT layer during consolidation,", .FALSE.  
 "Include sediment diagenesis processes,", .TRUE.  
 "Number of regions for different initial sediment concentrations,", 1  
 "Starting segment for regions,", 2  
 "Ending segment for regions,", 4  
 "Initial temperature for each region C,", 20.0  
 "Initial particulate organic carbon (total) concentration for each region  
 mgC/l,", 0.0  
 "Initial particulate organic nitrogen (total) concentration for each region  
 mgN/l,", 0.0  
 "Initial sulfate concentration for each region mgS/l,", 0.0  
 "Initial dissolved ammonia concentration for each region mgN/l,", 0.0  
 "Initial total phosphate concentration for each region mgP/l,", 0.0  
 "Initial dissolved sulfide concentration for each region mgS/l,", 0.0  
 "Initial dissolved methane concentration for each region mgC/l,", 0.0  
 "Initial total inorganic carbon concentration for each region mgC/l,", 11.9  
 "Initial alkalinity concentration for each region mg/l as CaCO<sub>3</sub>", 40.0  
 "Initial Ferrous Iron concentration for each region mgFe/l,", 1.0  
 "Initial Iron Oxyhydroxide concentration for each region mgFe/l,", 1.0  
 "Initial Mn(II) concentration for each region mgMn/l,", 1.0  
 "Initial manganese dioxide concentration for each region mgMn/l,", 1.0  
 "Include generic sediment BOD constituents,", .TRUE.  
 "Number of generic sediment BOD constituents,", 3  
 "Generic sediment BOD constituent names,", "SBOD1","SBOD2","SBOD3"  
 "Number of regions for initializing generic sediment BOD constituents,", 1  
 "Starting segment for generic BOD initialization for each region,", 2  
 "Ending segment for generic BOD initialization for each region,", 4

"Initial concentration for generic BOD per region mg/l," ,0.0  
 "Initial concentration for generic BOD per region mg/l," ,0.0  
 "Initial concentration for generic BOD per region mg/l," ,0.0  
 "Number of regions for different generic sediment BOD constituent consumption rate," , 1  
 "Starting segment for generic BOD consumption for each region," , 2  
 "Ending segment for generic BOD consumption for each region," , 4  
 "Consumption rate for generic BOD per region 1/d," ,0.0  
 "Consumption rate for generic BOD per region 1/d," ,0.0  
 "Consumption rate for generic BOD per region 1/d," ,0.0  
 "Temperature coefficient for generic BOD decay per region," ,1.01  
 "Temperature coefficient for generic BOD decay per region," ,1.02  
 "Temperature coefficient for generic BOD decay per region," ,1.03  
 "Number of regions for different diagenesis related rates," , 1  
 "Starting segment for regions," , 2  
 "Ending segment for regions," , 4  
 "Fraction of labile poc for each diagenesis region," ,0.65  
 "Fraction of refractory poc for each diagenesis region," ,0.25  
 "Fraction of labile pon for each diagenesis region," ,0.65  
 "Fraction of refractory pon for each diagenesis region," ,0.2  
 "Pore water diffusion coefficient m<sup>2</sup>/d," ,0.0005  
 "DO Threshold for aerobic layer oxidation rates mgO<sub>2</sub>/l," ,2.0  
 "Nitrification rate in aerobic layer (NH<sub>3</sub>->NO<sub>3</sub>) at DO below threshold m/d," ,0.131  
 "Nitrification rate in aerobic layer (NH<sub>3</sub>->NO<sub>3</sub>) at DO above threshold m/d," ,0.131  
 "Denitrification rate in aerobic layer (NO<sub>3</sub>->N<sub>2</sub>) at DO below threshold m/d," ,0.1  
 "Denitrification rate in aerobic layer (NO<sub>3</sub>->N<sub>2</sub>) at DO above threshold m/d," ,0.25  
 "Denitrification rate in anerobic layer (NO<sub>3</sub>->N<sub>2</sub>) m/d," ,0.25  
 "Methane oxidation rate in aerobic layer m/d," ,0.0  
 "Nitrification half-saturation constant for NH<sub>4</sub>N in aerobic layer mgN/l," ,0.728  
 "Nitrification half-saturation constant for O<sub>2</sub> in aerobic layer mgO<sub>2</sub>/l," ,0.37  
 "Temperature coefficient for pore water diffusion between layers," ,1.08  
 "Temperature coefficient for nitrification," ,1.123  
 "Temperature coefficient for denitrification," ,1.08  
 "Temperature coefficient for methane oxidation," ,1.079  
 "Sulfate concentration above which sulfide over methane is produced mgS/l," ,20.0  
 "Sulfide oxidation rate in aerobic layer m/d," ,0.0  
 "Temperature coefficient for sulfide oxidation," ,1.08  
 "Sulfide oxidation normalization constant for O<sub>2</sub> mgO<sub>2</sub>/l," ,4.0  
 "Mineralization rate for labile PON 1/d," ,0.035  
 "Mineralization rate for refractory PON 1/d," ,0.035  
 "Mineralization rate for inert/slow refractory PON 1/d," ,0.035  
 "Mineralization rate for labile POC 1/d," ,0.035  
 "Mineralization rate for refractory POC 1/d," ,0.035  
 "Mineralization rate for inert/slow refractory POC 1/d," ,0.035  
 "Mineralization rate for labile POP 1/d," ,0.035  
 "Mineralization rate for refractory POP 1/d," ,0.035

"Mineralization rate for inert/slow refractory POP 1/d," ,0.035  
 "Temperature coefficient for labile PON," ,1.1  
 "Temperature coefficient refractory PON," ,1.15  
 "Temperature coefficient inert/slow refractory PON," ,1.17  
 "Temperature coefficient labile POC," ,1.1  
 "Temperature coefficient refractory POC," ,1.15  
 "Temperature coefficient for inert/slow refractory POC," ,1.17  
 "Temperature coefficient labile POP," ,1.1  
 "Temperature coefficient refractory POP," ,1.15  
 "Temperature coefficient for inert/slow refractory POP," ,1.17  
 "Methane production calculation method (0: Analytical, 1: Numerical)," , 1  
 "Equilibrium constant for NH4+ <-> NH3 ionization. Provide as pK," , 9.1  
 "Equilibrium constant for HS- <-> H2S ionization. Provide as pK," , 9.0  
 "Henry's constant for NH3d <-> NH3g in atm/M," , 0.0179  
 "Henry's constant for CH4d <-> CH4g in atm/M," , 469  
 "Henry's constant for H2Sd <-> H2Sg in atm/M," , 10  
 "Henry's constant for CO2d <-> CO2g in atm/M," , 29  
 "Gas diffusion coefficient in sediment in m<sup>2</sup>/s," , 1.0d-9  
 "Calibration parameter R1 in m," , 0.0014  
 "Young's modulus E in N/m<sup>2</sup>," , 1.4d+9  
 "Critical stress intensity factor for sediments K1c in N/m<sup>3/2</sup>," , 300  
 "Bubbles release scale," , 0.02  
 "Fraction of critical pressure at which cracks close," , 0.20  
 "Switch to limit bubble size," , .TRUE.  
 "Maximum bubble radius in mm," , 80  
 "Switch to use slow release of bubbles," , .TRUE.  
 "Bubbles release fraction (sediments)," , 0.005  
 "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," ,.TRUE.  
 "Turbulence scaling factor for bubbles release," ,0.001  
 "Coefficient Bturb in Aturb\*ln(TSS) + Bturb = ln(Turbidity)," , -0.294  
 "Coefficient Aturb in Aturb\*ln(TSS) + Bturb = ln(Turbidity)," ,1.243  
 "Write sediment fluxes," , .TRUE.  
 "Oxygen stoichiometry for H2S decay in water column," ,1.88  
 "Oxygen stoichiometry for CH4 decay in water column," ,5.33  
 "Phosphorus Sorption Coefficient in Aerobic Layer m<sup>3</sup>/g," ,0.00005  
 "Phosphorus Sorption Coefficient in Anaerobic Layer m<sup>3</sup>/g," ,0.01  
 "Particle Mixing Velocity between Aerobic and Anaerobic Layers m/d," , 0.05  
 "Burial Velocity m/d," , 0.001  
 "Half-saturation constant for O2 for FeOOH reduction to Fe(II) g/m<sup>3</sup>," , 0.2  
 "Reduction rate, FeOOH to Fe(II) d-1," , 4.0  
 "Oxidation rate, Fe(II) to FeOOH m<sup>3</sup>/d-g," , 1.0  
 "FeOOH Settling Velocity m/d," , 0.001  
 "Fe(II) Sorption Coefficient in Aerobic Layer m<sup>3</sup>/g," ,0.00005  
 "Fe(II) Sorption Coefficient in Anaerobic Layer m<sup>3</sup>/g," ,0.01  
 "Oxygen stoichiometry for Fe(II) decay gO/gFe," ,0.143

"Half-saturation constant for O2 for MnO2 reduction to Mn(II) g/m<sup>3</sup>", 0.2  
 "Reduction rate, MnO2 to Mn(II) d<sup>-1</sup>", 0.002  
 "Oxidation rate, Mn(II) to MnO2 m<sup>3</sup>/d-g", 0.0001  
 "MnO2 Settling Velocity m/d", 0.001  
 "Mn(II) Sorption Coefficient in Aerobic Layer m<sup>3</sup>/g", 0.00005  
 "Mn(II) Sorption Coefficient in Anaerobic Layer m<sup>3</sup>/g", 0.01  
 "Oxygen stoichiometry for Mn(II) decay gO/gMn, ", 0.291

## W2\_CEMA\_Input.npt Input Descriptions

### Line Comments

Lines that begin with a dollar sign '\$' are skipped by the model when reading the input file. In the sample input file the first 3 lines are skipped.

Sample Line	Description
\$Additional CEMA related W2 input	Line Comment
\$Please see help file for input description	Line Comment
\$All lines starting with \$ are comments and disregarded by the model	Line Comment

### Constituent Numbers

Some of the constituents included in the OSPLM are not modeled in the standard CE-QUAL-W2 model. These constituents occupy spots in the constituent order normally occupied by generic constituents.

Sample Line	Description
"H2S Constituent Number (Generic Constituent)", 2	Constituent number for hydrogen sulfide
"CH4 Constituent Number (Generic Constituent)", 3	Constituent number for methane
"SO4 Constituent Number (Generic Constituent)", 4	Constituent number for sulfate
"Turbidity Constituent Number (Generic Constituent)", 6	Constituent number for turbidity
"Fe(II) Constituent Number (Generic Constituent)", 7	Constituent number of ferrous Iron Fe(II)
"FeOOH Constituent Number (Generic Constituent)", 8	Constituent number of Iron Oxyhydroxide FeOOH
"Mn(II) Constituent Number (Generic Constituent)", 9	Constituent number of Manganese Mn(II)
"MnO2 Constituent Number (Generic Constituent)", 10	Constituent number of Manganese Dioxide MnO2

### Bed Consolidation

Sample Line	Description
"Switch to perform bed consolidation," .FALSE.	Switch to perform bed consolidation. '.TRUE.' or '.FALSE.'
"Fraction of layer thickness at which water layer is added," 1.0	Fraction of layer thickness at which water layer is added
"Number of bed consolidation regions," 1	Number of bed consolidation regions
"Starting segment for regions," 2	Starting segment for regions
"Ending segment for regions," 4	Ending segment for regions
"Data type for bed consolidation for each region (0: Constant, 1: Time varying)," 1	Data type for bed consolidation for each region
"Bed consolidation rate (m/d)," 0.02739726	Bed consolidation rate (m/d)
"Bed consolidation data file," "Regn1.npt,"	Bed consolidation data file

### Initial Conditions

Sample Line	Description
"Initial bed elevation in meters," 0.1	Initial bed elevation (m)
"Initial sediment bed porosity," 0.8	Initial sediment bed porosity
"Maximum Water Surface Elevation," 10.0	Maximum Water Surface Elevation (m). Used to determine width of sediment diagnosis zone beneath water column
"Initial Porewater Temperature (C)," 20.0	Initial Porewater Temperature (°C)

### Sediment Characteristics

Sample Line	Description
"Sediment bed particle size in microns," 100	Sediment bed particle size (microns)
"Sediment type 1: Cohesive, 2: Non-cohesive," 2	Sediment type: '1'=Cohesive, '2'= Noncohesive
"Sediment bulk density (kg/m <sup>3</sup> )," 2600	Sediment bulk density (kg/m <sup>3</sup> )
"Sediment particle settling velocity (m/d)," 5.0	Sediment particle settling velocity (m/d)
"Include sediment resuspension and deposition processes," .TRUE.	Switch to include sediment resuspension and deposition processes. '.TRUE.' or '.FALSE.'



### Consolidation Output

Sample Line	Description
"Write bed elevation snapshot output," .TRUE.	Switch to write bed elevation snapshot output. '.TRUE.' or '.FALSE.'
"Write bed porosity snapshot output," .TRUE.	Switch to write bed porosity snapshot output. '.TRUE.' or '.FALSE.'

### Fine Fluids Tailing (FFT) Layer

Sample Line	Description
"Include FFT Layer," .FALSE.	Switch to include FFT Layer. '.TRUE.' or '.FALSE.'
"FFT Layer Number of Periods," 5	FFT Layer Number of Periods
"FFT Layer Start Times," 1,65,125,200,300	FFT Layer Start Times (Julian Day)
"FFT Layer End Times," 50,100,175,250,400	FFT Layer End Times (Julian Day)
"Initial tailings concentration in FFT (gm/m <sup>3</sup> )," 360000	Initial tailings concentration in FFT (g/m <sup>3</sup> )
"Settling velocity of FFT to MFT (m/d)," 0.d0	Settling velocity of FFT to MFT (m/d)
"Move FFT layer during consolidation," .FALSE.	Switch to move FFT layer during consolidation. '.TRUE.' or '.FALSE.'

### Diagenesis Initial Conditions

Sample Line	Description
"Include sediment diagenesis processes," .TRUE.	Switch to include sediment diagenesis processes
"Number of regions for different initial sediment concentrations," 1	Number of regions for different initial sediment concentrations
"Starting segment for regions," 2	Starting segment for regions
"Ending segment for regions," 4	Ending segment for regions
"Initial temperature for each region C," 20.0	
"Initial particulate organic carbon (total) concentration for each region mgC/l," 0.0	Initial particulate organic carbon (total) concentration for each region (mgC/l)
"Initial particulate organic nitrogen (total) concentration for each region mgN/l," 0.0	Initial particulate organic nitrogen (total) concentration for each region (mgN/l)
"Initial sulfate concentration for each region mgS/l," 0.0	Initial sulfate concentration for each region (mg-S/l)

Sample Line	Description
"Initial dissolved ammonia concentration for each region mgN/l,", 0.0	Initial dissolved ammonia concentration for each region (mg-N/l)
"Initial total phosphate concentration for each region mgP/l,", 0.0	Initial dissolved sulfide concentration for each region (mg-P/l)
"Initial dissolved sulfide concentration for each region mgS/l,", 0.0	Initial dissolved sulfide concentration for each region (mg-S/l)
"Initial dissolved methane concentration for each region mgC/l,", 0.0	Initial dissolved methane concentration for each region (mg-C/l)
"Initial total inorganic carbon concentration for each region mgC/l,", 11.9	Initial total inorganic carbon concentration for each region (mg-C/l)
"Initial alkalinity concentration for each region mg/l as CaCO3,", 40.0	Initial alkalinity concentration for each region (mg-CaCO3/l)
"Initial Ferrous Iron concentration for each region mgFe/l,", 1.0	Initial ferrous iron concentration for each region (mg-Fe/l)
"Initial Iron Oxyhydroxide concentration for each region mgFe/l,", 1.0	Initial iron oxyhydroxide concentration for each region (mg-Fe/l)
"Initial Mn(II) concentration for each region mgMn/l,", 1.0	Initial Mn(II) concentration for each region (mg-Mn/l)
"Initial manganese dioxide concentration for each region mgMn/l,", 1.0	Initial manganese dioxide concentration for each region (mg-Mn/l)

### *Generic BOD Constituent Settings*

Sample Line	Description
"Include generic sediment BOD constituents,", .TRUE.	Switch to include generic BOD constituents in sediments
"Number of generic sediment BOD constituents,", 3	Number of generic BOD constituents
"Generic sediment BOD constituent names,", "SBOD1", "SBOD2", "SBOD3"	Generic BOD constituent names
"Number of regions for initializing generic sediment BOD constituents,", 1	Number of regions for different initial generic BOD concentrations
"Starting segment for generic BOD initialization for each region,", 2	Starting segment for regions
"Ending segment for generic BOD initialization for each region,", 4	Ending segment for regions
"Initial concentration for generic BOD per region mg/l,", 0.0	Initial generic BOD concentration for each region (mg/l)
"Initial concentration for generic BOD per region mg/l,", 0.0	Initial generic BOD concentration for each region (mg/l)

Sample Line	Description
"Initial concentration for generic BOD per region mg/l," ,0.0	Initial generic BOD concentration for each region (mg/l)

### *Generic BOD Rate Settings*

Sample Line	Description
"Number of regions for different generic sediment BOD constituent consumption rate," , 1	Number of regions for different generic BOD consumption rates
"Starting segment for generic BOD consumption for each region," , 2	Starting segment for regions
"Ending segment for generic BOD consumption for each region," , 4	Ending segment for regions
"Consumption rate for generic BOD per region 1/d," ,0.0	Generic BOD consumption rate for each region (1/d)
"Consumption rate for generic BOD per region 1/d," ,0.0	Generic BOD consumption rate for each region (1/d)
"Consumption rate for generic BOD per region 1/d," ,0.0	Generic BOD consumption rate for each region (1/d)
"Temperature coefficient for generic BOD decay per region," ,1.01	Generic BOD temperature coefficient for each region
"Temperature coefficient for generic BOD decay per region," ,1.02	Generic BOD temperature coefficient for each region
"Temperature coefficient for generic BOD decay per region," ,1.03	Generic BOD temperature coefficient for each region

### *Diagenesis Region Settings*

Sample Line	Description
"Number of regions for different diagenesis related rates," , 1	Number of regions for different diagenesis related rates
"Starting segment for regions," , 2	Starting segment for regions
"Ending segment for regions," , 4	Ending segment for regions
"Fraction of labile poc for each diagenesis region," ,0.65	Fraction of labile POC for each diagenesis region
"Fraction of refractory poc for each diagenesis region," ,0.25	Fraction of refractory POC for each diagenesis region
"Fraction of labile pon for each diagenesis region," ,0.65	Fraction of labile PON for each diagenesis region
"Fraction of refractory pon for each diagenesis region," ,0.2	Fraction of refractory PON for each diagenesis region

### Diagenesis Rates Settings Part 1

Sample Line	Description
"Pore water diffusion coefficient m <sup>2</sup> /d, ", 0.0005	Porewater diffusion coefficient (m <sup>2</sup> /d)
"DO Threshold for aerobic layer oxidation rates mgO <sub>2</sub> /l, ", 2.0	DO Threshold for aerobic layer oxidation rates (mgO <sub>2</sub> /l)
"Nitrification rate in aerobic layer (NH <sub>3</sub> ->NO <sub>3</sub> ) at DO below threshold m/d, ", 0.131	Nitrification rate in aerobic layer (NH <sub>3</sub> ->NO <sub>3</sub> ) at DO below threshold (m/d)
"Nitrification rate in aerobic layer (NH <sub>3</sub> ->NO <sub>3</sub> ) at DO above threshold m/d, ", 0.131	Nitrification rate in aerobic layer (NH <sub>3</sub> ->NO <sub>3</sub> ) at DO above threshold (m/d)
"Denitrification rate in aerobic layer (NO <sub>3</sub> ->N <sub>2</sub> ) at DO below threshold m/d, ", 0.1	Denitrification rate in aerobic layer (NO <sub>3</sub> ->N <sub>2</sub> ) at DO below threshold (m/d)
"Denitrification rate in aerobic layer (NO <sub>3</sub> ->N <sub>2</sub> ) at DO above threshold m/d, ", 0.25	Denitrification rate in aerobic layer (NO <sub>3</sub> ->N <sub>2</sub> ) at DO above threshold (m/d)
"Denitrification rate in anerobic layer (NO <sub>3</sub> ->N <sub>2</sub> ) m/d, ", 0.25	Denitrification rate in anerobic layer (NO <sub>3</sub> ->N <sub>2</sub> ) (m/d)
"Methane oxidation rate in aerobic layer m/d, ", 0.0	Methane oxidation rate in erobic layer (m/d)
"Nitrification half-saturation constant for NH <sub>4</sub> N in aerobic layer mgN/l, ", 0.728	Nitrification half-saturation constant for NH <sub>4</sub> N in aerobic layer (mgN/l)
"Nitrification half-saturation constant for O <sub>2</sub> in aerobic layer mgO <sub>2</sub> /l, ", 0.37	Nitrification half-saturation constant for O <sub>2</sub> in aerobic layer (mgO <sub>2</sub> /l)

### Diagenesis Rates Settings Part 2

Sample Line	Description
"Temperature coefficient for pore water diffusion between layers, ", 1.08	Temperature coefficient for porewater diffusion between layers
"Temperature coefficient for nitrification, ", 1.123	Temperature coefficient for nitrification
"Temperature coefficient for denitrification, ", 1.08	Temperature coefficient for denitrification
"Temperature coefficient for methane oxidation, ", 1.079	Temperature coefficient for methane oxidation
"Sulfate concentration above which sulfide over methane is produced mgS/l, ", 20.0	Sulfate concentration above which sulfide over methane is produced (mgS/l)
"Sulfide oxidation rate in aerobic layer m/d, ", 0.2	Sulfide oxidation rate in zerobic layer m/d
"Temperature coefficient for sulfide oxidation, ", 1.08	Temperature coefficient for sulfide oxidation
"Sulfide oxidation normalization constant for O <sub>2</sub> mgO <sub>2</sub> /l, ", 4.0	Sulfide oxidation normalization constant for O <sub>2</sub> (mgO <sub>2</sub> /l)

Sample Line	Description
"Mineralization rate for labile PON 1/d," ,0.035	Mineralization rate for labile PON (1/d)
"Mineralization rate for refractory PON 1/d," ,0.035	Mineralization rate for refractory PON (1/d)

### **Diagenesis Rates Settings Part 3**

Sample Line	Description
"Mineralization rate for inert/slow refractory PON 1/d," ,0.035	Mineralization rate for inert/slow refractory PON (1/d)
"Mineralization rate for labile POC 1/d," ,0.035	Mineralization rate for labile POC (1/d)
"Mineralization rate for refractory POC 1/d," ,0.035	Mineralization rate for refractory POC (1/d)
"Mineralization rate for inert/slow refractory POC 1/d," ,0.035	Mineralization rate for inert/slow refractory POC (1/d)
"Mineralization rate for labile POP 1/d," ,0.035	Mineralization rate for labile POP (1/d)
"Mineralization rate for refractory POP 1/d," ,0.035	Mineralization rate for refractory POP (1/d)
"Mineralization rate for inert/slow refractory POP 1/d," ,0.035	Mineralization rate for inert/slow refractory POP (1/d)
"Temperature coefficient for labile PON," ,1.1	Temperature coefficient for labile PON
"Temperature coefficient refractory PON," ,1.15	Temperature coefficient refractory PON
"Temperature coefficient inert/slow refractory PON," ,1.17	Temperature coefficient inert/slow refractory PON

### **Diagenesis Rates Settings Part 4**

Sample Line	Description
"Temperature coefficient labile POC," ,1.1	Temperature coefficient labile POC
"Temperature coefficient refractory POC," ,1.15	Temperature coefficient refractory POC
"Temperature coefficient for inert/slow refractory POC," ,1.17	Temperature coefficient for inert/slow refractory POC
"Temperature coefficient labile POP," ,1.1	Temperature coefficient labile POP
"Temperature coefficient refractory POP," ,1.15	Temperature coefficient refractory POP
"Temperature coefficient for inert/slow refractory POP," ,1.17	Temperature coefficient for inert/slow refractory POP

### Methane Calculation Setting

Sample Line	Description
"Methane production calculation method (0: Analytical, 1: Numerical)," , 1	Methane production calculation method (0: Analytical, 1: Numerical)

### Ionization Settings

Sample Line	Description
"Equilibrium constant for NH <sub>4</sub> <sup>+</sup> <-> NH <sub>3</sub> ionization. Provide as pK," , 9.1	Equilibrium constant for NH <sub>4</sub> <sup>+</sup> <-> NH <sub>3</sub> ionization. Provide as pK
"Equilibrium constant for HS <sup>-</sup> <-> H <sub>2</sub> S ionization. Provide as pK," , 9.0	Equilibrium constant for HS <sup>-</sup> <-> H <sub>2</sub> S ionization. Provide as pK

### Dissolution Settings

Sample Line	Description
"Henry's constant for NH <sub>3</sub> d <-> NH <sub>3</sub> g in atm/M," , 0.0179	Henry's constant for NH <sub>3</sub> d <-> NH <sub>3</sub> g (atm/M)
"Henry's constant for CH <sub>4</sub> d <-> CH <sub>4</sub> g in atm/M," , 469	Henry's constant for CH <sub>4</sub> d <-> CH <sub>4</sub> g (atm/M)
"Henry's constant for H <sub>2</sub> Sd <-> H <sub>2</sub> Sg in atm/M," , 10	Henry's constant for H <sub>2</sub> Sd <-> H <sub>2</sub> Sg (atm/M)
"Henry's constant for CO <sub>2</sub> d <-> CO <sub>2</sub> g in atm/M," , 29	Henry's constant for CO <sub>2</sub> d <-> CO <sub>2</sub> g (atm/M)

### Gas Bubble Formation Rates

Sample Line	Description
"Gas diffusion coefficient in sediment in m <sup>2</sup> /s," , 1.0d-9	Gas diffusion coefficient in sediment (m <sup>2</sup> /s)
"Calibration parameter R1 in m," , 0.0014	Calibration parameter R1 (m)
"Young's modulus E in N/m <sup>2</sup> ," , 1.4d+9	Young's modulus E (N/m <sup>2</sup> )
"Critical stress intensity factor for sediments K <sub>1c</sub> in N/m <sup>3/2</sup> ," , 300	Critical stress intensity factor for sediments K <sub>1c</sub> (N/m <sup>3/2</sup> )
"Bubbles release scale," , 0.02	Bubbles release scale
"Fraction of critical pressure at which cracks close," , 0.20	Fraction of critical pressure at which cracks close
"Switch to limit bubble size," , .TRUE.	Switch to limit bubble size
"Maximum bubble radius in mm," , 80	Maximum bubble radius (mm)
"Switch to use slow release of bubbles," , .TRUE.	Switch to use slow release of bubbles
"Bubbles release fraction (sediments)," , 0.005	Bubbles release fraction (sediments)
"Bubbles accumulation fraction," , 0.1	Bubbles accumulation fraction
"Number of bubbles release array," , 2000	Number of bubbles release array

Sample Line	Description
"Bubbles release fraction (atmosphere),", 0.001	Bubbles release fraction (atmosphere)
"Bubbles-Water gas exchange rate (1/s),", 1.0d-7	Bubbles-Water gas exchange rate (1/s)

### Bubble Related Turbulence

Sample Line	Description
"Apply additional turbulence due to bubbles release,", .TRUE.	Apply additional turbulence due to bubbles release, '.TRUE.' or '.FALSE.'
"Turbulence scaling factor for bubbles release,", 0.001	Scaling factor for bubbles related turbulence

### Turbidity Calculations

Sample Line	Description
"Coefficient Bturb in Aturb*ln(TSS) + Bturb = ln(Turbidity),", -0.294	Coefficient Aturb in turb*ln(TSS) + Bturb = ln(Turbidity)
"Coefficient Aturb in Aturb*ln(TSS) + Bturb = ln(Turbidity),", 1.243	Coefficient Bturb in Aturb*ln(TSS) + Bturb = ln(Turbidity)

### Sediment Flux Output Settings

Sample Line	Description
"Write sediment fluxes,", .TRUE.	Switch to write sediment fluxes, '.TRUE.' or '.FALSE.'

### Additional Diagenesis Rate Settings, Particle Velocities and Kinetic Parameters

Sample Line	Description
"Oxygen stoichiometry for H2S decay in water column,", 1.88	Oxygen stoichiometry for hydrogen sulfide decay in water column, g-O2/ g-S
"Oxygen stoichiometry for CH4 decay in water column,", 5.33	Oxygen stoichiometry for methane decay in water column, g-O2/ g-C
"Phosphorus Sorption Coefficient in Aerobic Layer m <sup>3</sup> /g", 0.00005	Phosphorus sorption coefficient in the aerobic layer, m <sup>3</sup> g <sup>-1</sup>
"Phosphorus Sorption Coefficient in Anaerobic Layer m <sup>3</sup> /g", 0.01	Phosphorus sorption coefficient in the anaerobic layer, m <sup>3</sup> g <sup>-1</sup>
"Particle Mixing Velocity between Aerobic and Anaerobic Layers m/d", 0.05	Particle Mixing Velocity between Aerobic and Anaerobic Layers m/d
"Burial Velocity m/d", 0.001	Burial Velocity of sediments, m/d
"Half-saturation constant for O2 for FeOOH reduction to Fe(II) g/m <sup>3</sup> ", 0.2	Half-saturation constant for O2 for FeOOH reduction to Fe(II) g/m <sup>3</sup>
"Reduction rate, FeOOH to Fe(II) d <sup>-1</sup> ", 4.0	Iron Oxyhydroxide (FeOOH) Reduction rate, d <sup>-1</sup>

Sample Line	Description
"Oxidation rate, Fe(II) to FeOOH m <sup>3</sup> /d-g", 1.0	Oxidation rate of Ferrous Iron or Fe(II) , m <sup>3</sup> d <sup>-1</sup> g <sup>-1</sup>
"FeOOH Settling Velocity m/d", 0.001	Iron Oxyhydroxide (FeOOH) Settling Velocity, m/d
"Fe(II) Sorption Coefficient in Aerobic Layer m <sup>3</sup> /g",0.00005	Fe(II) sorption coefficient in aerobic Layer, m <sup>3</sup> /g
"Fe(II) Sorption Coefficient in Anaerobic Layer m <sup>3</sup> /g",0.01	Fe(II) sorption coefficient in anaerobic Layer m <sup>3</sup> /g
"Oxygen stoichiometry for Fe(II) decay gO/gFe, ",0.143	Oxygen stoichiometry for Fe(II) decay g-O/g-Fe
"Half-saturation constant for O <sub>2</sub> for MnO <sub>2</sub> reduction to Mn(II) g/m <sup>3</sup> ", 0.2	Half-saturation constant of oxygen for manganese dioxide reduction, g/m <sup>3</sup>
"Reduction rate, MnO <sub>2</sub> to Mn(II) d <sup>-1</sup> ", 0.002	Reduction rate of manganese dioxide, d <sup>-1</sup>
"Oxidation rate, Mn(II) to MnO <sub>2</sub> m <sup>3</sup> /d-g", 0.0001	Oxidation rate of manganese, m <sup>3</sup> /d-g
"MnO <sub>2</sub> Settling Velocity m/d", 0.001	Manganese dioxide settling velocity, m/d
"Mn(II) Sorption Coefficient in Aerobic Layer m <sup>3</sup> /g",0.00005	Manganese sorption coefficient in aerobic layer, m <sup>3</sup> /g
"Mn(II) Sorption Coefficient in Anaerobic Layer m <sup>3</sup> /g",0.01	Manganese sorption coefficient in anaerobic layer, m <sup>3</sup> /g
"Oxygen stoichiometry for Mn(II) decay gO/gMn, ",0.291	Oxygen stoichiometry for manganese decay, gO/gMn

### pH\_buffering.npt and w2\_con.npt input files:

Description of file inputs for the pH and alkalinity routines have been adapted from Sullivan et al. (2013).

The change to the W2 control file are additional flags to turn ON/OFF the enhanced pH and non-conservative alkalinity subroutines.

The variables PHBUFC turns ON/OFF the use of enhanced pH buffering and NALKC turns ON/OFF the use of non-conservative alkalinity.

#### Example:

```
MISCELL      NDAY SELECTC HABTATC ENVIRPC AERATEC INITUWL PHBUFC NCALKC
              100      OFF      OFF      OFF      OFF      OFF      ON      ON
```

An example pH\_buffering.npt file is shown below.

#### Example:



## Enhanced pH Buffering Input File for CE-QUAL-W2

BUFTYPE	NH4BUFC	PO4BUFC	OMBUFC						
	ON	ON	ON						
OM TYPE	OMTYPE	NAG	POMBUFC						
	DIST	2	OFF						
DENSITY	SDEN	SDEN	SDEN	SDEN	SDEN	SDEN	SDEN	SDEN	SDEN
	0.14	0.10							
pK VALS	PK	PK	PK	PK	PK	PK	PK	PK	PK
	4.5	9.6							
STD DEV	PKSD	PDSD	PDSD	PDSD	PDSD	PDSD	PDSD	PDSD	PDSD
	1.2	1.0							

pH\_buffering.npt variable descriptions (Sullivan et al., 2013):

NH4BUFC: ON/OFF, specifies whether ammonia/ammonium is included in pH buffering

PO4BUFC: ON/OFF, specifies whether phosphoric acid is included in pH buffering

OMBUFC: ON/OFF, specifies whether organic matter is included in pH buffering

OMTYPE: DIST or MONO where DIST specifies one or more Gaussian distributions of pKa values, or MONO specifies a collection of discrete pKa values

NAG: number of acid/base groups to model, either as the means of Gaussian distributions of pKa values or as discrete monoprotic acids

POMBUFC: ON/OFF, specifies whether POM is included in OM buffering where ON indicates that OM buffering includes both DOM and POM. OFF indicates that OM buffering includes only DOM

SDEN: site density, in moles of acid/base sites per mole of carbon in OM

PK: the pKa values (negative log10 of the acid dissociation constant), specified either as the mean of a distribution or a discrete value

PKSD: the standard deviation for a Gaussian distribution of pKa values (ignored when specifying an OMTYPE of MONO)

## Bed Consolidation Rate Input File

If desired, the user can specify the bed consolidation rate. Input file names are specified by the user in W2\_CEMA\_Input.npt. The bed consolidation rate input file is a time series input file with a column header line that is skipped. Additional comment lines can be added at the beginning of the file if they begin with a '\$'.

**Example:**

\$Bed consolidation (m/d) rate

JDay      Consolidation

1.000 0.01370

2.000 0.01370

3.000 0.01370

4.000 0.01370

5.000 0.01370

6.000 0.01370

## Appendix C – Example Application: Wahiawa Reservoir

Wahiawa Reservoir, Figure 15, is a freshwater reservoir located in central Oahu, Hawaii. The reservoir has 2 forks which converge at the dam as shown in Figure 2. The north fork is about 5.23 km (3.25 miles) and the south fork is about 8.45 km (5.25 miles). The dam was built in 1906 by Waialua Sugar Company to provide irrigation water for sugar cane fields. Since 1928 Wahiawa sewage treatment plant has discharged effluent into Wahiawa Reservoir. Another treatment plant, Whitmore Village, discharged into the North Fork of Wahiawa starting in 1969. Currently, only the Wahiawa Treatment Plant discharges to the reservoir.

The reservoir has an average depth of about 8 m (26.2 ft) and a maximum depth of 27 m (98.5 ft) at the dam. The reservoir occupies 121.4 ha (300 acres), and the spillway crest is at 256.8 m MSL (842.5 ft MSL). The dam has multiple withdrawal outlets, but over the last couple of decades only the bottom one at a center line elevation of 236.31 m MSL (775.3 ft MSL) has been used.

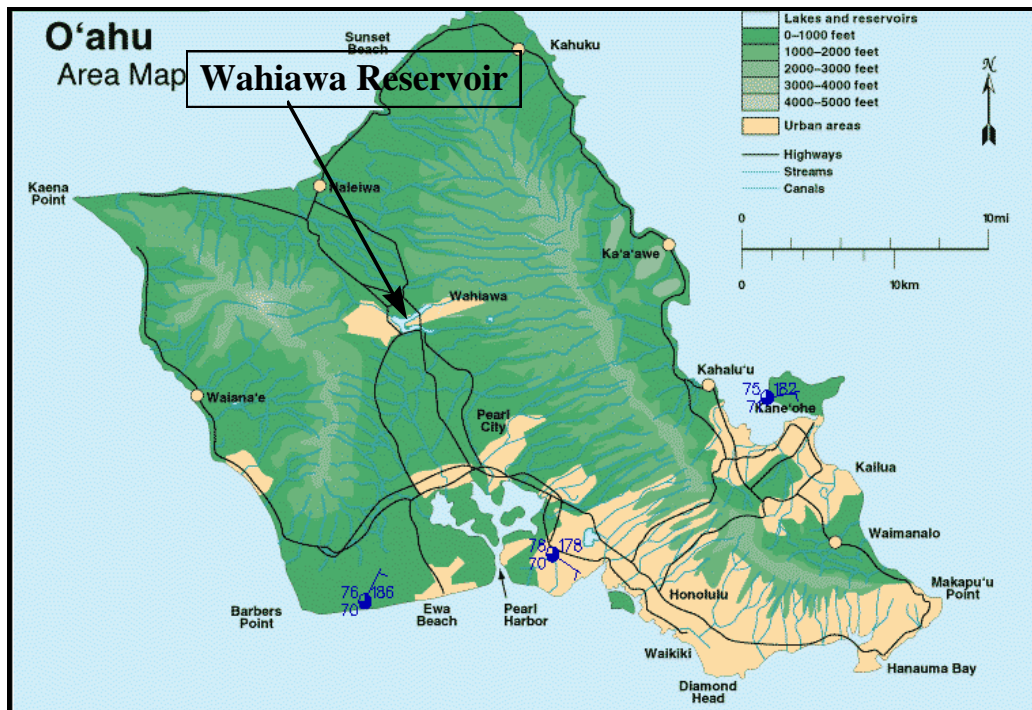


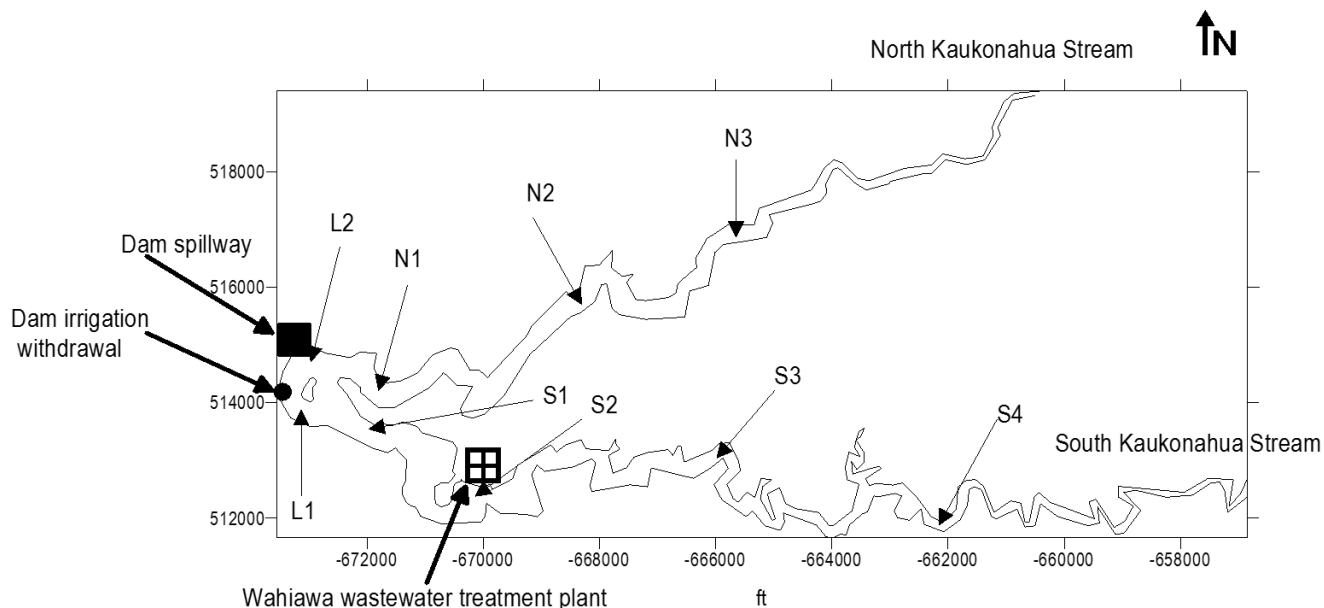
Figure 15 Wahiawa Reservoir, Oahu, Hawaii.

Several previous studies of Wahiawa Reservoir were performed in the 1970's. These studies showed that accelerated eutrophication of Wahiawa Reservoir was a serious problem. Major fish kills were reported in 1962, 1968, 1971, and 1975 as a result of little or no dissolved oxygen in the reservoir. These kills were attributed to anoxia resulting from reservoir drawdown to a level where oxygen was not present (the rate of sediment oxygen demand and other sinks were greater than algal production and reaeration). Current field data (1995, 1996) have shown that about 40% of the volume of the reservoir is always below 4 mg/l. The reservoir is stratified most of the year with supersaturated oxygen conditions at the reservoir surface

and an anoxic hypolimnion. Since the reservoir rarely turns over, new oxygen to the hypolimnion is from oxygenated inflows only.

## Model Set-Up

The model has 2 branches as shown in Figure 16. Details of the bathymetry are shown in Table 6.



**Figure 16. Wahiawa Reservoir sampling stations.**

**Table 6 Model branch characteristics.**

Branch	Length (ft)	Length (m)	Segment spacing, ft	Segment spacing, m	Number of model segments	Segment number upstream end	Segment number downstream end
1	25314	7716	844	257	30	2	31
2	17675	5387	884	269	20	34	53

The model grid is shown in Figure 17 and Figure 18. The vertical grid spacing was 0.61 m.

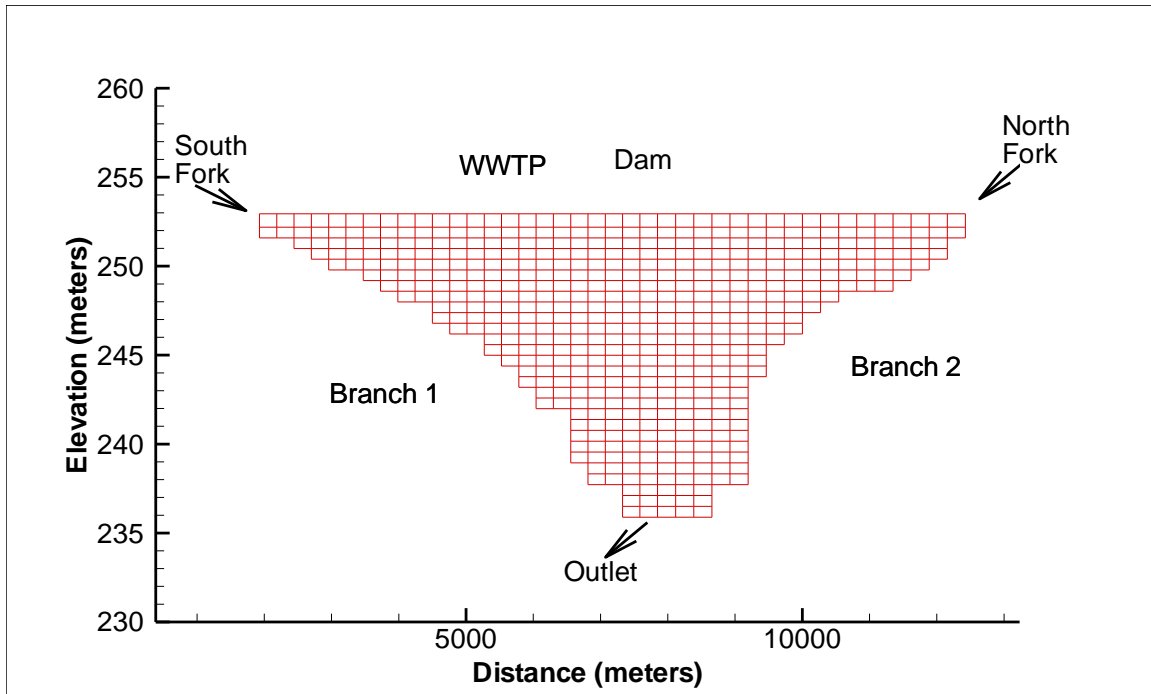


Figure 17. Wahiawa Reservoir Model Grid.

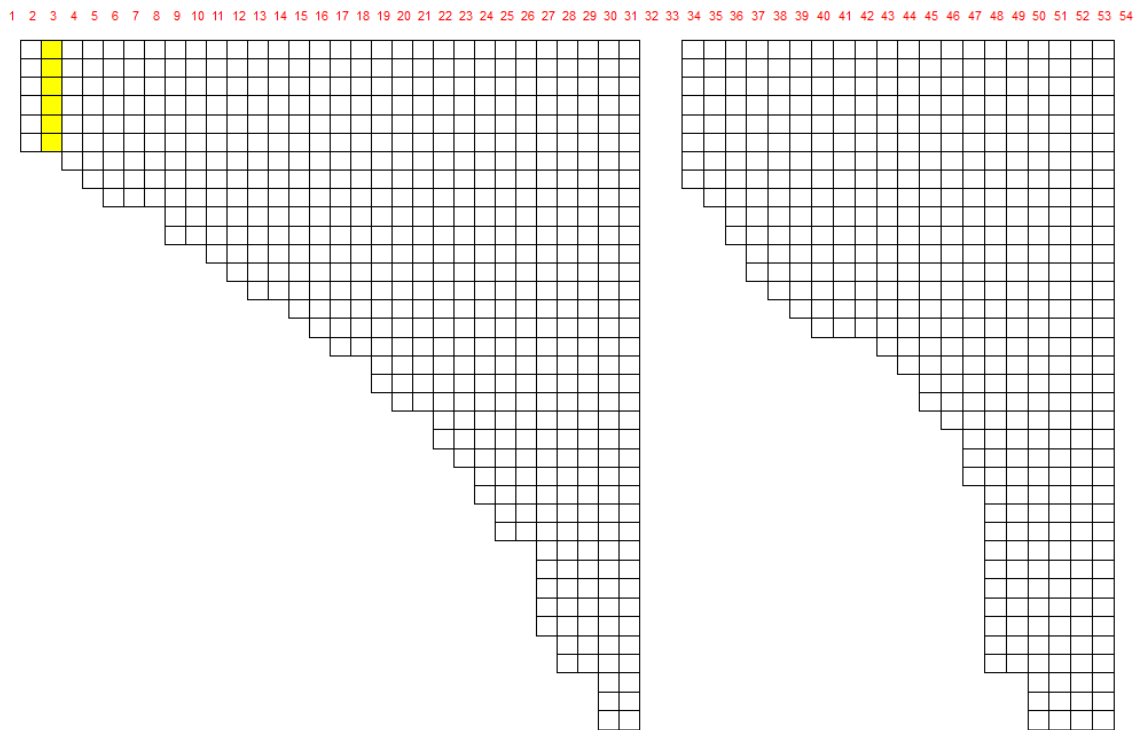


Figure 18. Model side view of 2 branches.

The location of the inflows and outflows is shown in Table 7.

**Table 7. Model segment numbers for inflows and outflows.**

Inflow/Outflow	Segment number
South Kaukaonahua Stream	2
North Kaukaonahua Stream	33
Wastewater treatment plant	25
Dam outfall	31

## Boundary Conditions

Inflows to Wahiawa reservoir are from the Wahiawa wastewater treatment plant (see Table 8), the North and South forks of the Kaukonahua Stream (see Table 9), and ungaged storm water inflows through storm water pipes distributed along the reservoir. Outflow is through the bottom outlet of the selective withdrawal structure for irrigation and over the spillway when the water levels are high. Meteorological data are typical of tropical conditions as shown in Table 10.

**Table 8. Typical water quality characteristics of the wastewater treatment plant effluent.**

DO mg/l	ammonia mg/l	nitrate- nitrite mg/l	Total N mg/l	ortho- phosphate mg/l	Total P mg/l	TSS mg/l	Flow cfs
2	17	.05	20	1.5	2	20	3.0

**Table 9. Typical water quality and flow characteristics of North Fork Kaukonahua and South Fork Kaukonahua streams.**

Inflow	D.O. mg/l	ammonia mg/l	nitrate- nitrite, mg/l	Total N mg/l	ortho- Phosphate, mg/l	Total P mg/l	TSS mg/l	Flow cfs*
N. Fork- USGS gage 2000	7	.02	.2	.6	.01	.03	10	14
S. Fork- USGS gage 2080	7	.01	.5	1.5	.01	.05	10	17

\* N. and S. Fork were USGS measurements at a gaging station several miles upstream of the reservoir sections

**Table 10. Typical meteorological conditions at Honolulu International Airport between April 1995 and February 1996.**

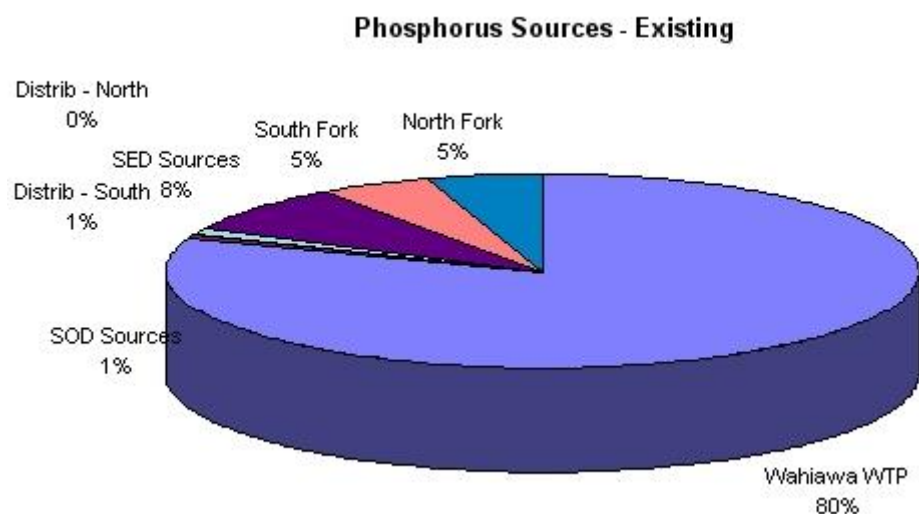
Parameter	Air Temperature, C	Dew Point Temperature , C	Cloud Cover, tenths	Wind Speed, meters/secon d	Relative humidity, percent	Equilibrium temperature, C
Mean	26.4	20.1	5.1	4.9	69.4	23.0

Standard deviation	3.1	1.9	3.2	2.2	12.2	3.5
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## Big Picture System Look

Field data and model observations have shown the following:

- Wahiawa WWTP is the primary source of the algal limiting nutrient P (see Figure 19). Sediment release of P is inhibited because of P-deficient clays entering the reservoir from the South fork. These clays effectively bind P and “bury” it in the sediment. Note that CE-QUAL-W2 cannot selectively inhibit P release from the sediments unless one makes some minor source code changes. [Note that in Figures 5-7 SOD is the fixed sediment oxygen demand rate as a function of longitudinal cell and SED is the first order sediment decay that is set to zero at the beginning of the simulation.]



**Figure 19** Sources of P for Wahiawa Reservoir.

- the reservoir is dominated by plunging inflows from the 2 tributaries which short circuit the reservoir and cause water in the photic zone to have very long detention times (this is particularly important considering that the Wahiawa WWTP discharges to the surface)
- respiring algae and sediment oxygen demand are the primary sources of ammonia release (which could be the accumulation of decades of WWTP discharge) and oxygen uptake (see Figure 20). The hypolimnion routinely violates ammonia toxicity standards.
- sediment oxygen demand dominates the oxygen consumption (see Figure 21)
- the discharge from the Wahiawa WWTP has a tremendous impact on the photic zone and the growth of algae because of its surface discharge. Also, the effluent from the Wahiawa WWTP moves upstream on the Southern arm because of the plunging inflows (this was verified by field data taken during 1995 and 1996).

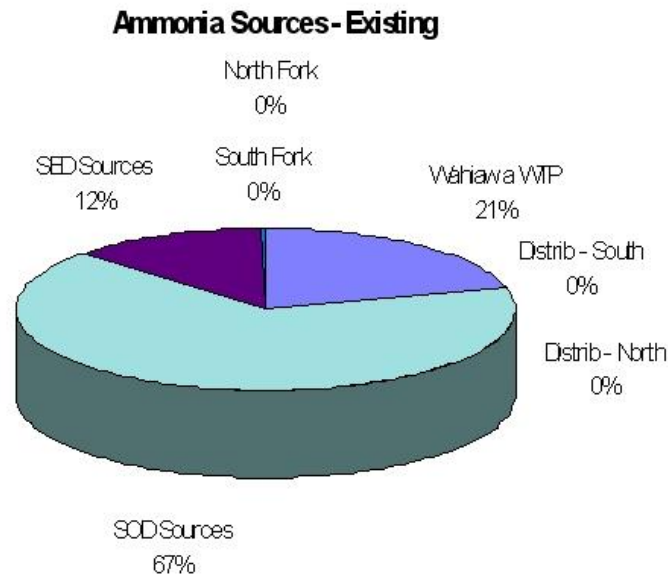


Figure 20. Ammonia sources for Wahiawa Reservoir.

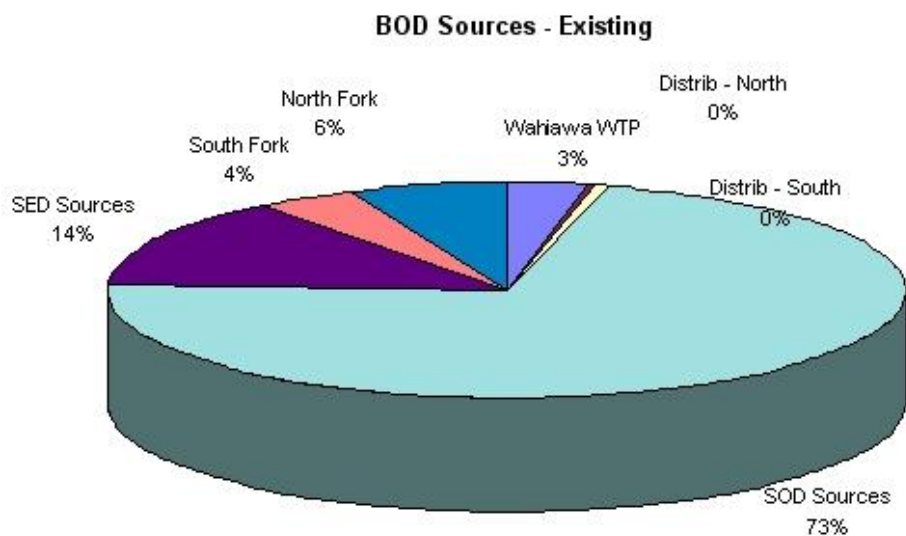


Figure 21 BOD sources in Wahiawa Reservoir.

## Sediment Diagenesis Module

The sediment diagenesis module consists of an aerobic layer and an anaerobic layer. Constituents modeled are shown in Figure 22. The sediment diagenesis module predicts dissolved oxygen demand of the sediments and also predicts the mass transfer of ammonia, phosphate, methane, hydrogen sulfide, carbon dioxide and DO to and from the water column. Once transferred from the sediments, hydrogen sulfide and methane can oxidize in the water column and exerting further DO demand



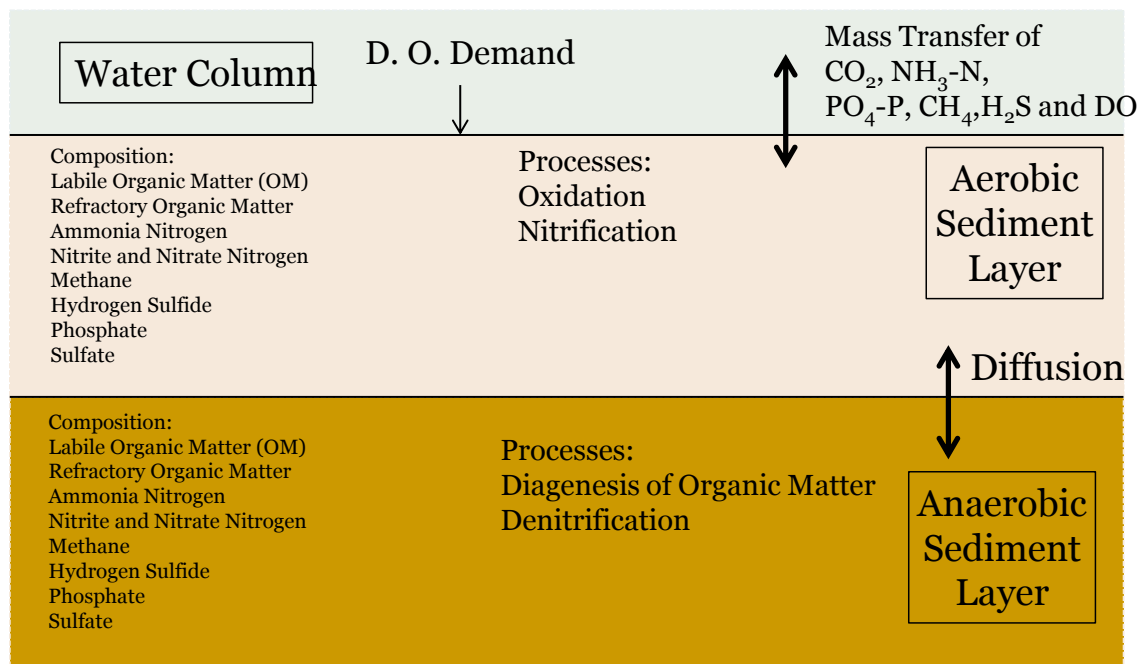


Figure 22. Model sediment diagenesis processes in Wahiawa Reservoir model.

## Running the Model

Before turning on the sediment diagenesis model the existing zeroth order and first order sediment compartments need to be turned off. The first order compartment can be turned off by setting the control file parameter SEDC to OFF. The zeroth order compartment can be turned off by setting all the segment specific SOD values in the control file to zero. A simpler approach is to set FSOD, which is the fraction of zeroth order SOD rate used, to zero.

The switch to turn on the sediment diagenesis model is located in the input file 'W2\_CEMA\_Input.npt'. New input files used by the sediment diagenesis model are listed in Table 4. These files are described in detail in the appendix. 'W2\_CEMA\_Input.npt' is a comma delimited text file that can be edited using a text editor. The module can be turned on by going to line 40 and setting value of the logical variable to '.TRUE.':

```
"Settling velocity of FFT to MFT (m/d)", 0.d0
"Move FFT layer during consolidation", .FALSE.
"Include sediment diagenesis processes", .TRUE.
"Number of regions for different initial sediment concentrations", 1
"Starting segment for regions", 2
"Ending segment for regions", 53
```

To have the model generate the time and volume averaged DO and chlorophyll a concentrations, turn on the environmental performance criterion feature (set ENVIRPC to 'ON' in control file). Check the

environmental performance criteria input file w2\_envirprf.npt to make sure that DO and chlorophyll a are set to 'ON'. Run the model by double clicking on 'w2\_ivf64.exe'.

Record some of the overall statistics about chlorophyll a concentration (see output file envrprf\_cd.dat) and dissolved oxygen (see output file envrprf\_c.dat). An example of the 'envrprf\_c.dat' output file is shown below:

```
"      DOinterval" "Fraction of volume"
20.00      0.0000E+00
19.00      0.0000E+00
18.00      0.0000E+00
17.00      0.0000E+00
16.00      0.0000E+00
15.00      0.1424E-04
14.00      0.1470E-03
13.00      0.7181E-03
12.00      0.2798E-02
11.00      0.1005E-01
10.00      0.3626E-01
 9.00      0.9802E-01
 8.00      0.1439E+00
 7.00      0.1078E+00
 6.00      0.7525E-01
 5.00      0.5248E-01
 4.00      0.4595E-01
 3.00      0.4382E-01
 2.00      0.4500E-01
 1.00      0.3378E+00

0      0.1000E+01

0      0.4864E+01
```

The temporal and spatial average of DO is located in the lower right corner and is highlighted.

Particulate organic carbon (POC), particulate organic nitrogen (PON), and particulate organic phosphorus (POP) each consist of a fast decaying (labile), a slow decaying (refractory), and very slow decaying (inert) components. Mineralization rates can be specified in the 'W2\_CEMA\_input.npt' file starting at line 87:

```
"Mineralization rate for labile PON 1/d," ,0.12
"Mineralization rate for refractory PON 1/d," ,0.001
"Mineralization rate for inert/slow refractory PON 1/d," ,0.00001
"Mineralization rate for labile POC 1/d," ,0.12
"Mineralization rate for refractory POC 1/d," ,0.001
```

```
"Mineralization rate for inert/slow refractory POC 1/d,",0.00001
"Mineralization rate for labile POP 1/d,",0.12
"Mineralization rate for refractory POP 1/d,",0.001
"Mineralization rate for inert/slow refractory POP 1/d,",0.00001
```

Initial conditions for POC, PON, and POP are also specified in the 'W2\_CEMA\_input.npt' file starting at line 45:

```
Initial particulate organic carbon (total) concentration for each region
mgC/l,", 20000.0
"Initial particulate organic nitrogen (total) concentration for each
region mgN/l,", 500.0
"Initial particulate organic phosphorus (total) concentration for each
region mgP/l,",10.0
```

Their respective labile and refractory components are specified starting at line 63:

```
"Fraction of labile poc for each diagenesis region,",0.65
"Fraction of refractory poc for each diagenesis region,",0.25
"Fraction of labile pon for each diagenesis region,",0.65
"Fraction of refractory pon for each diagenesis region,",0.2
"Fraction of labile pop for each diagenesis region,",0.65
"Fraction of refractory pop for each diagenesis region,",0.2
```

Any remaining fraction is classified as inert.

The sediment oxygen demand predicted at each model segment is located in the output file 'SOD.opt'. The sediment particulate organic carbon concentration predicted for each segment is output to the file 'POC\_Sediments.opt'. PON, PON, methane and hydrogen sulfide concentrations in the sediments are written to the output files 'PON\_Sediments.opt', 'POP\_Sediments.opt', 'CH4\_Sediments.opt', and 'H2S\_Sediments.opt', respectively.

The sensitivity of DO and algae predictions in the water column to the initial sediment conditions can be investigated by changing the initial concentrations of particulate organic phosphorus (POP), particulate organic nitrogen (PON), and particulate organic carbon (POC) to different values. Table 11 shows the average reservoir dissolved oxygen and chlorophyll a concentrations with POP, PON, and POC initial conditions doubled and halved. Doubling initial conditions concentrations resulted in lower dissolved oxygen concentrations due to higher SOD. Algae (or chlorophyll a) concentrations increased due to the doubling initial of initial nutrient concentrations. Likewise, when initial sediment concentrations were halved, DO increased and algae concentrations decreased.

**Table 11. Model results.**

Statistic	Initial simulation	Initial sediment POC, PON, and POP concentrations doubled	Initial sediment POC, PON, and POP concentrations halved
Temporal and spatial volume weighted dissolved oxygen in the reservoir (mg/l)	4.86	4.71	5.02
Temporal and spatial volume weighted chlorophyll a concentration in the reservoir (ug/l)	43.0	52.5	37.1

Model input and output files are listed in Table 12 and Table 13, respectively.

**Table 12. Model input files.**

File Type	File Name	Description
control file	w2_con.npt	model control file
bathymetry file	bth.csv	segment lengths, initial water surface elevation, segment orientation, layer thicknesses and cell widths
graph file	graph.npt	This file controls input and output format.
meteorological file	met.npt	time series file containing temperature, dew point temperature, wind speed, wind direction and cloud cover data
initial condition files	lpr.npt	vertical/longitudinal initial temperatures and constituents
branch inflow files	qin_br1.npt	flow rate file for branch 1 inflow
	qin_br2.npt	flow rate file for branch 2 inflow
	tin_br1.npt	temperature file for branch 1 inflow
	tin_br2.npt	temperature file for branch 2 inflow
	cin_br1.npt	constituent file for branch 1 inflow
	cin_br2.npt	constituent file for branch 2 inflow
branch outflow files	Qot_br1.npt	flow rate file for branch 1 outflow (dam)
distributed tributary files	qdt_br1.npt	flow rate file for branch 1 distributed tributary
	qdt_br2.npt	flow rate file for branch 2 distributed tributary
	tdt_br1.npt	temperature file for branch 1 distributed tributary
	tdt_br2.npt	temperature file for branch 2 distributed tributary

File Type	File Name	Description
	cdt_br1.npt	constituent file for branch 1 distributed tributary
	cdt_br2.npt	constituent file for branch 2 distributed tributary
tributary file (WWTP)	qtr_tr1.npt	flow rate file for Wahiawa WTP
	ttr_tr1.npt	temperature file for Wahiawa WTP
	ctr_tr1.npt	constituent file for Wahiawa WTP
Shade file	Shade.npt	Shade information for each model segment
Wind sheltering file	Wsc.npt	Wind sheltering for each model segment
Aerator input file	w2_aerate.npt	Input parameters for using aerator feature
Environmental Performance Criteria Input File	w2_envirprf.npt	Input parameters for specifying environmental performance criteria
Habitat volume input file	w2_habitat.npt	Input parameters for calculating habitat volumes
Selective withdrawal input file	w2_selective.npt	Input parameters for selective withdrawal feature
Sediment diagenesis input files	W2_CEMA_Input.npt	setup for the all the CEMA related inputs except for those of the enhanced pH buffering and non-conservative alkalinity subroutines
	pH_buffering.npt	Inputs for enhanced pH buffering and non-conservative alkalinity subroutines (not used in this example problem)
	User specified bed consolidation rate file(s)	Time series file of bed consolidation rate (not used in this example problem)

**Table 13. Model output files.**

File Type	File Name	Description
model output files	snp.opt	snapshot file
	vpl.opt	vector file
	cpl.opt	contour file
	habitat3.opt	Habitat volume output file
	envrprf_t.dat	Environmental performance criteria output file for temperature
	envrprf_c.dat	Environmental performance criteria output file for constituents
	envrprf_cd.dat	Environmental performance criteria output file for derived constituents

	surfvoltavg.opt	Surface (upper 4 model layers) Volume weighted WQ parameters at specified segments
	volwgtavg.opt	Volume weighted WQ parameters at specified segments
	sodsed.opt	Time series output for zeroth order SOD plus first order sediment oxygen demand at all time and all segments
	qwo_31.opt	Combined outflow time series for segment 31 (dam segment)
	two_31opt	Combined outflow temperature time series for segment 31 (dam segment)
	cwo_31.opt	Combined outflow concentration time series for segment 31 (dam segment)
	qwo_str*_seg31.opt	Outflow file time series for structure at segment 31 (dam segment)
	two_str*_seg31.opt	Outflow temperature time series for structure located at segment 31 (dam segment)
	cwo_str*_seg31.opt	Outflow constituent time series for located at segment 31 (dam segment)
	vpl.w2l	Binary output file for W2_Tool Post-Processor
Sediment Diagenesis Output Files	SOD.opt	Sediment oxygen demand predicted at each model segment
	POC_Sediments.opt	Sediment particulate organic carbon concentration predicted for each segment
	PON_Sediments.opt	Sediment particulate organic nitrogen concentration predicted for each segment
	POP_Sediments.opt	Sediment particulate organic phosphorus concentration predicted for each segment
	CH4_Sediments.opt	Sediment methane concentration predicted for each segment
	H2S_Sediments.opt	Sediment hydrogen sulfide concentration predicted for each segment