CIEG 460/660 − Water Quality Modeling Spring 2006

Water Column - Sediment Two Layer Model

General Case

Water Column (1)

$$H_1 \frac{dC_{T1}}{dt} = -v_s f_{p1} C_{T1} + v_{rs} f_{p2} C_{T2} - v_d \left(f_{d1} C_{T1} - f_{d2} C_{T2} \right) - \frac{Q}{A} C_{T1} - k_1 H_1 C_{T1}$$

Sediment (2)

$$H_2 \frac{dC_{T2}}{dt} = +v_s f_{p1} C_{T1} - v_{rs} f_{p2} C_{T2} + v_d \left(f_{d1} C_{T1} - f_{d2} C_{T2} \right) - k_2 H_2 C_{T1} - v_b f_{p2} C_{T2}$$

Factored Equations

$$\frac{dC_{T1}}{dt} = -((v_s f_{p1} + v_d f_{d1})/H_1 + +k_1 + \frac{1}{t_0})C_{T1} + (v_{rs} f_{p2} + v_d f_{d2})/H_1 C_{T2}$$

$$\frac{dC_{T2}}{dt} = +(v_s f_{p1} + v_d f_{d1})/H_2 C_{T1} - ((v_{rs} f_{p2} + v_d f_{d2} + v_b f_{p2})/H_2 + k_2) C_{T2}$$

Simplified NotationEquations

$$\frac{dC_{T1}}{dt} = -s_1^{\prime} C_{T1} + s_2 \frac{H_2}{H_1} C_{T2}$$

$$\frac{dC_{T2}}{dt} = s_1 \frac{H_1}{H_2} C_{T1} - s_2^{\prime} C_{T2}$$

Definitions

$$s_1^{\prime} = s_1 + k_1 + \frac{1}{t_0}$$

$$s_2^{\prime} = s_2 + k_2 + v_b f_{p2}/H_2$$

Notation: primes denote s + reaction rates and transport out.

Gross Fluxes

$$j_{1\to 2} = v_s f_{p1} + v_d f_{d1}$$

$$j_{2\to 1} = v_{rs} f_{p2} + v_d f_{d2}$$

$$s_1 = \frac{j_{1\to 2}}{H_1}$$

$$s_2 = \frac{j_{2\to 1}}{H_2}$$

General Solution

$$C_{T1}(t) = C_{T1}(0)\left(\frac{s'_2 - g_1}{g_2 - g_1}\exp(-g_1 t) - \frac{s'_2 - g_2}{g_2 - g_1}\exp(-g_2 t)\right) + C_{T2}(0)\frac{H_2}{H_1}\frac{s_2}{g_2 - g_1}\left(\exp(-g_1 t) - \exp(-g_2 t)\right)$$

$$C_{T2}(t) = C_{T2}(0)\left(\frac{s'_1 - g_1}{g_2 - g_1}\exp(-g_1 t) - \frac{s'_1 - g_2}{g_2 - g_1}\exp(-g_2 t)\right) + C_{T1}(0)\frac{H_1}{H_2}\frac{s_1}{g_2 - g_1}\left(\exp(-g_1 t) - \exp(-g_2 t)\right)$$

where

$$\left.\begin{matrix} g_1 \\ g_2 \end{matrix}\right\} = \frac{1}{2}\left(s'_1 + s'_2\right)\left(1 \pm \left(1 - \frac{4(s'_1 s'_2 - s_1 s_2)}{\left(s'_1 + s'_2\right)^2}\right)^{1/2}\right)$$

Approximate Inverse Time Constants
Using

$$\sqrt{1-\varepsilon} = 1 - \frac{\varepsilon}{2} + \cdots$$

and since

$$1 \gg \frac{4(s'_1 s'_2 - s_1 s_2)}{\left(s'_1 + s'_2\right)^2}$$

the result is

$$g_1 \simeq s'_1 + s'_2$$

which is the large time constant (sum of all loss rates)

$$g_2 \simeq \frac{s'_1 s'_2 - s_1 s_2}{s'_1 + s'_2}$$

which is the small time constant (difference over a sum)
Water Column Concentration

$$C_{T1}(t) \simeq C_{T1}(0)\left(\frac{s'_2}{s'_1 + s'_2}\exp(-g_2 t) + \frac{s'_1}{s'_1 + s'_2}\exp(-g_1 t)\right) C_{T2}(0)\frac{H_2}{H_1}\frac{s_2}{s'_1 + s'_2}\left(\exp(-g_2 t) - \exp(-g_1 t)\right)$$

Sediment Concentration

$$
\begin{aligned}
C_{T2}(t) \quad \simeq \quad & C_{T2}(0)\left(\frac{s_1'}{s_1' + s_2'}\exp(-g_2 t) + \frac{s_2'}{s_1' + s_2'}\exp(-g_1 t)\right) \\
& C_{T1}(0)\frac{H_1}{H_2}\frac{s_1}{s_1' + s_2'}\left(\exp(-g_2 t) - \exp(-g_1 t)\right)
\end{aligned}
$$

Note that solutions are completely symmetric wrt $1 \leftrightarrow 2$

Examine solution for $C_{T2}(0) = 0$.After the fast time constant decays to zero, $\exp(-g_1 t) \to 0$, the solution is

$$
\frac{C_{T2}(t)}{C_{T1}(t)} = \frac{H_1}{H_2}\frac{s_1}{s_2'} = \frac{v_s f_{p1} + v_d f_{d1}}{v_{rs} f_{p2} + v_b f_{p2} + v_d f_{d2} + k_2 H_2}
$$

Express solution as r_2/r_1

$$
\frac{r_2}{r_1} = \frac{C_{p2}/m_2}{C_{p1}/m_1} = \frac{f_{p2} C_{T2}/m_2}{f_{p1} C_{T1}/m_1} = \frac{f_{p2}}{f_{p1}}\frac{m_1}{m_2}\left(\frac{v_s f_{p1} + v_d f_{d1}}{v_{rs} f_{p2} + v_b f_{p2} + v_d f_{d2} + k_2 H_2}\right)
$$

Now first term:

$$
\frac{f_{p2}}{f_{p1}}\frac{m_1}{m_2}\left(v_s f_{p1}\right)
$$

using sediment solids mass balance

$$
m_1 v_s = m_2\left(v_{rs} + v_b\right)
$$

$$
\frac{m_1}{m_2} = \frac{v_{rs} + v_b}{v_s}
$$

yields

$$
\frac{f_{p2}}{f_{p1}}\frac{m_1}{m_2}\left(v_s f_{p1}\right) = \left(v_{rs} + v_b\right) f_{p2}
$$

Second term

$$
\frac{f_{p2}}{f_{p1}}\frac{m_1}{m_2}\left(v_d f_{d1}\right)
$$

Using

$$
f_{d1} = \frac{1}{1 + m_1 K_{p1}} \qquad f_{p1} = \frac{m_1 K_{p1}}{1 + m_1 K_{p1}}
$$

So

$$
\begin{aligned}
\frac{f_{p2}}{f_{p1}}\frac{m_1}{m_2} v_d f_{d1} \quad &= \quad \frac{f_{d1}}{f_{p1}}\frac{m_1}{m_2} v_d f_{p2} = \frac{1}{m_1 K_{p1}}\frac{m_1}{m_2} v_d f_{p2} \\
&= \quad \frac{1}{m_1 K_{p1}}\frac{m_1}{m_2} v_d \frac{m_2 K_{p2}}{1 + m_2 K_{p2}} = \frac{K_{p2}}{K_{p1}} v_d f_{d2}
\end{aligned}
$$

Finally

$$
\frac{r_2}{r_1} = \frac{\left(v_{rs} + v_b\right) f_{p2} + \dfrac{K_{p2}}{K_{p1}} v_d f_{d2}}{\left(v_{rs} + v_b\right) f_{p2} + v_d f_{d2} + k_2 H_2}
$$

which is the steady state r_2/r_1

Slow inverse time constant

$$g_2 \simeq \frac{s_1' s_2' - s_1 s_2}{s_1' + s_2'}$$

Numerator

$$\begin{aligned} s_1' s_2' - s_1 s_2 &= (s_1 + k_1')(s_2 + k_2') - s_1 s_2 \\ &= s_1 s_2 + k_1' s_2 + k_2' s_1 + k_1' k_2' - s_1 s_2 \\ &= k_1' s_2 + k_2' s_1 + k_1' k_2' \\ &= k_1' s_2' + k_2' s_1 \end{aligned}$$

where

$$\begin{aligned} k_1' &= k_1 + \frac{1}{t_0} \\ k_2' &= k_2 + \frac{v_b f_{p2}}{H_2} \end{aligned}$$

Therefore

$$g_2 = \frac{k_1' s_2' + k_2' s_1}{s_1' + s_2'} = \frac{s_2'}{s_1' + s_2'} \left(k_1' + k_2' \frac{s_1}{s_2'} \right)$$

and

$$\frac{s_1}{s_2'} = \frac{H_2}{H_1} \frac{C_{T2}}{C_{T1}}$$

so that

$$g_2 = \frac{s_2'}{s_1' + s_2'} \left(k_1' + \frac{H_2}{H_1} \frac{C_{T2}}{C_{T1}} k_2' \right)$$

and using r_2/r_1

$$g_2 = \frac{s_2'}{s_1' + s_2'} \left(k_1' + \beta \frac{r_2}{r_1} k_2' \right)$$