Introduction to (Great Lakes) Water Quality Modeling

Ecosystem Restoration Workshop

June 2008

Basic idea

- Based on fundamental "truths", usually stated in terms of conservation of a particular property
  - e.g. mass, momentum, energy
    - Mass is neither created nor destroyed, but may change form
    - Momentum is governed by certain physical laws (such as Newton's laws), reacts to forces
    - Energy also is conserved, but may change form, such as potential ⇔ kinetic

- Most physical models based on rate expressions –
  - For example, consider the process of filling a tank with water; how would you answer the question, “What is the volume of water in the tank at any given time?”
    - The rate at which water is being added to (or leaking from) the tank should, intuitively, be part of the answer
    - In general, some initial starting point (initial condition) also needs to be known in order to calculate a history of water volume

- Formalization of problem in mathematical terms –
  - We can't start with V (volume) = ______ , since we don't know enough to start with
  - What do we know?
    - [Rate of change of V] = [filling rate] – [leaking rate]

$$\frac{dV}{dt} = Q_{in} - Q_{out}$$

(Q = flowrate)

$$\frac{dV}{dt} = Q_{in} - Q_{out}$$

- This is a simple first-order initial value problem, which can be solved if we know the flow values and initial condition
  - Let the initial volume be V_0
  - Assume the inflow rate is constant
  - Assume the outflow rate is proportional to V
  - Then,

$$Q_{out} = kV \qquad \frac{dV}{dt} + kV = Q_{in}$$

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- With the above assumptions, and if k is approximately constant (in reality it is a function of V), this equation happens to have an analytical solution
- More complicated problems that may not have an analytical solution are usually solved using numerical integration

Concentration changes

- Now consider the problem of changing concentration of a particular substance in a reactor (jar, tank, stream, lake, etc.);

  - [rate of change of mass] =

    [rate of transport in]

    - [rate of transport out]

    + (-) [net rate of transformation or production]

Note concept of <u>control volume</u> used here; also, “transport” includes both advective and diffusive processes.

Mathematical statement

$$\frac{dM}{dt} = \frac{d(CV)}{dt} = (QC)_{in} - (QC)_{out} - w_s CA - KCV$$

(+ dispersion)

M =	mass
C =	concentration
w_s =	settling rate (if applicable)
A =	bottom area
K =	first-order decay (growth) rate (if applicable)

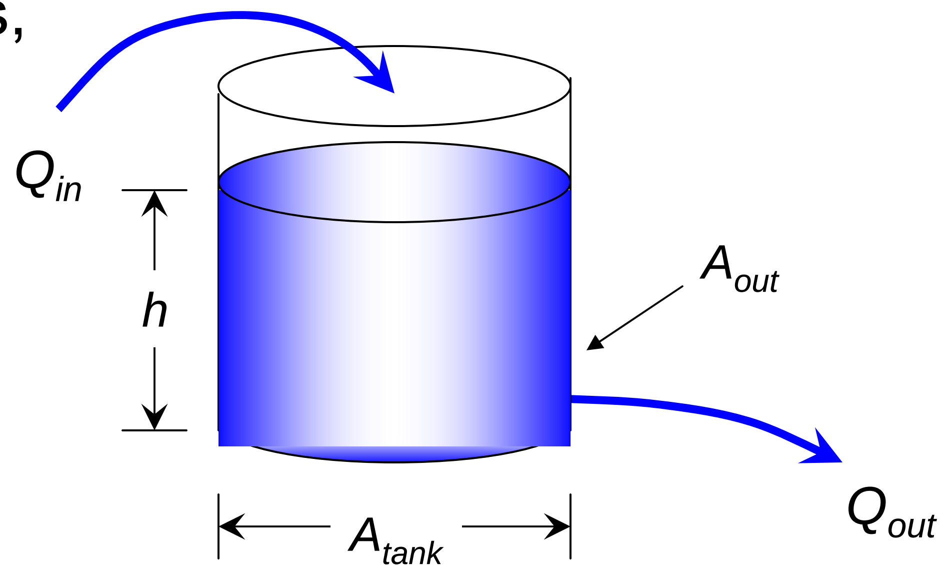
Stella application

- Tank filling example:

Recall $$\frac{dV}{dt} + kV = Q_{in}$$

From basic application of energy and mass conservation principles,

$$k \cong \sqrt{\frac{2g}{h}} \frac{A_{out}}{A_{tank}}$$



- If *h* is assumed to change only very slowly, then *k* is approximately constant (*k* is really a function of *V*) and an analytical solution may be obtained,

$$V \cong V_0 e^{-kt} + \frac{Q_{in}}{k}$$

- A steady state solution is found when d/dt $\rightarrow$ 0 or $t \rightarrow \infty$,

$$V_{steady} = \frac{Q_{in}}{k}$$

Numerical solution

- (perhaps better in this case, since fewer approximations)
- write

$$\frac{dV}{dt} + kV = Q_{in} \quad \Rightarrow dV = dt\underbrace{\left(Q_{in} - kV\right)}_{\text{rate}}$$

$$V_{i+1} = V_i + dt * \left(Q_{in} - k_i V_i\right)$$

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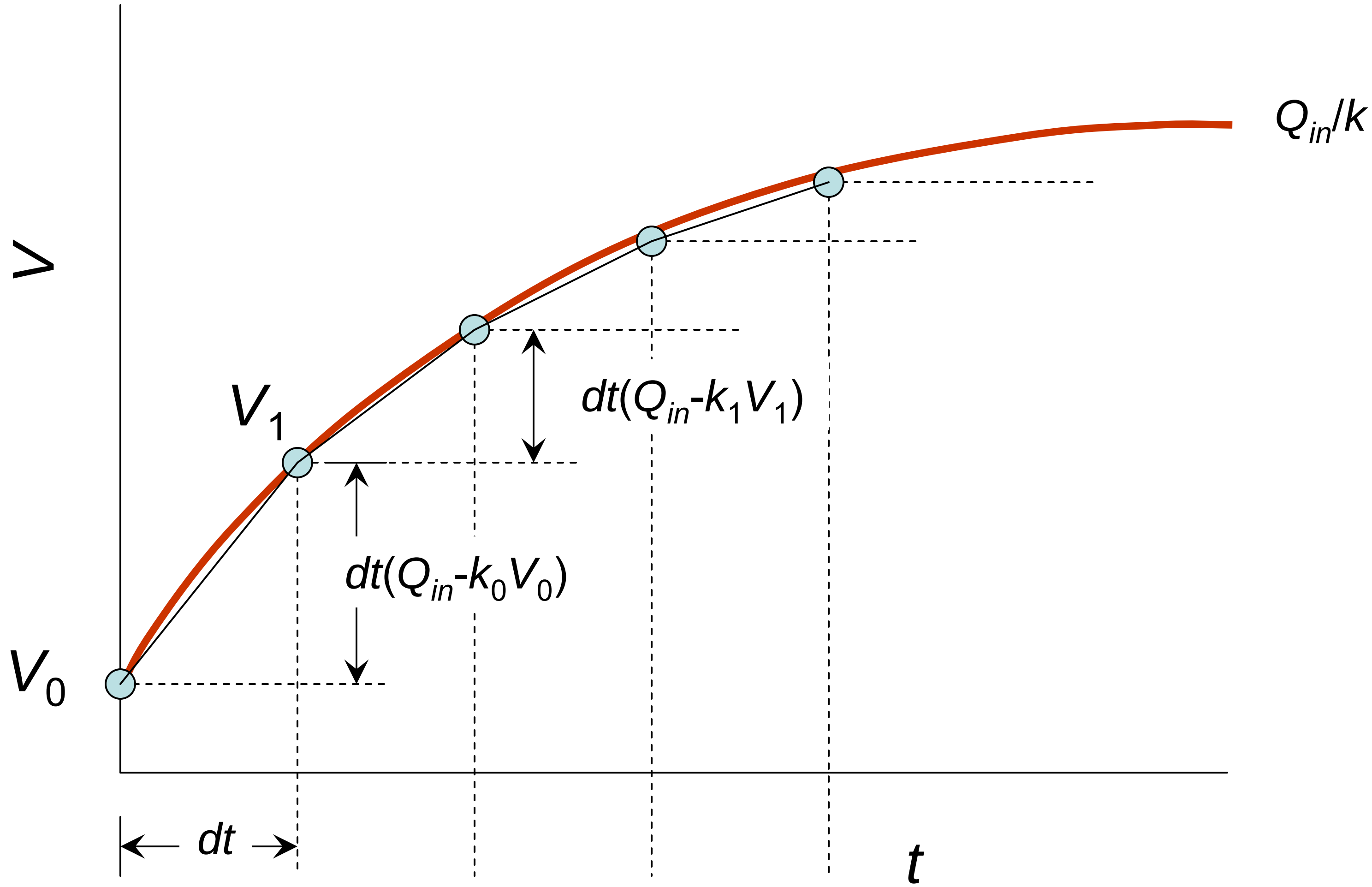


Concentration model

- Now consider the issue of changing concentration, still in a mixed reactor
  - From before, assume Q_{in} = Q_{out} = Q (so, V is constant)

$$\frac{dM}{dt} = \frac{d(CV)}{dt} = \boxed{(QC)_{in}} - (QC)_{out} - w_s CA - KCV$$

Often called loading, *W*

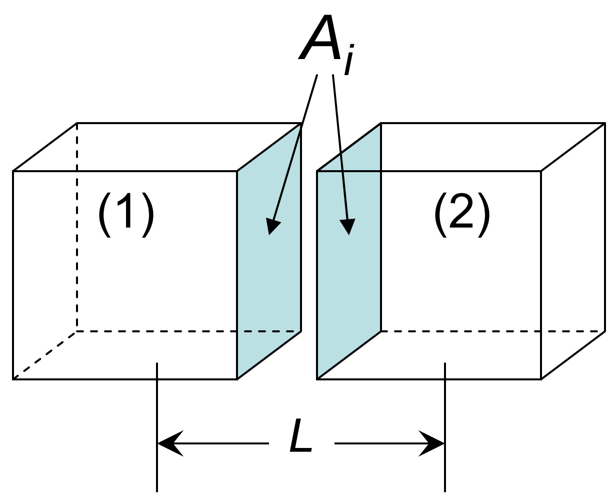
$$\frac{dC}{dt} = \frac{QC_{in}}{V} - C\frac{(Q + w_s A + KV)}{V}$$

$$\Rightarrow C = C_0 e^{-\lambda t} + \frac{QC_{in}}{\lambda V}, \quad \lambda = \frac{Q + w_s}{V} + K$$

(for constant coefficients)

Multiple reactors

- Add dispersion to account for exchange between reactors
  - Dispersive transport:
    L = distance over which change in C occurs (usually taken as distance between centers of reactors)
    A_i = interfacial area between reactors, over which dispersion occurs
    E' = bulk dispersion coefficient



$$\frac{E\,A_i}{L}\left(C_2 - C_1\right) = E'\left(C_2 - C_1\right)$$

Example applications

- Two reactors consist of Lake Huron and Saginaw Bay
  - Assuming steady state, estimate the exchange coefficient value *E'* using data from Table 1 (handout) for chloride

$$V_2 \frac{dC_2}{dt} = W_2 - Q_2 C_2 + E'\left(C_1 - C_2\right)$$

  - Formulate the full unsteady model (in Stella) and ensure that it reproduces the steady state concentrations

Ref: Chapra, Steven C., Surface Water Quality Modeling, McGraw-Hill, 1997

- Consider a model for Lake Erie that is based on a division of the lake into its three main basins (see Figure 1 on handout). Develop a model for phosphorus in the three basins using data from Table1 (handout).
  - You will need to choose settling velocities to try to match the data shown in Table 2 (handout).