Generals of Water Quality Modeling

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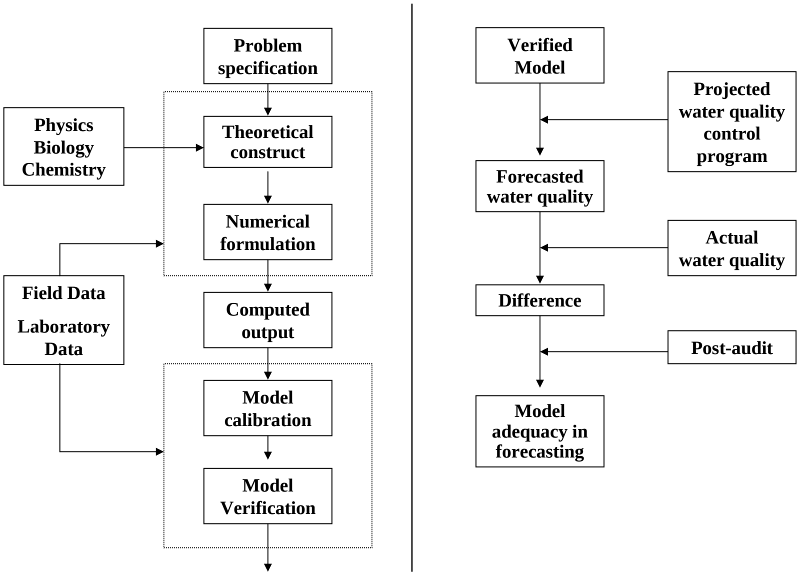
Water Quality Modeling

Why Water Quality Modeling?

- **Analysis**
  - **Understand Physical and Biochemical Reactions Occurred in Pollutant Transport**
  - **Where do all the chemicals go? How Rapidly are They Degrade?**
  - **Pollutants Influx Procedure into the Stream and Reservoir**
- **Predictions**
  - **Temporal & Spatial Water Quality Variation?**
  - **Water Quality Variations in the Reservoir Downstream Due to the Discharge Release**
  - **Water Quality Degradation In the Reservoir During Flood**
- **Evaluations**
  - **Reaction Evaluation to Meet the Target Concentration**
  - **Water Quality Due to Waste Load Reduction or Increase**
  - **Best Management Practice (BMP)**

Framework of Water Quality Modeling



Problem specification

Physics Biology Chemistry

Theoretical construct

Numerical formulation

Field Data

Laboratory Data

Computed output

Model calibration

Model Verification

Verified Model

Projected water quality control program

Forecasted water quality

Actual water quality

Difference

Post-audit

Model adequacy in forecasting

WATER QUALITY MODELING

GOAL

To predict the response of a water body to some external stimulus.

Example:

For a linear system we could write

$$\boxed{\text{Response} = \frac{W}{\P}}$$

where:
W is a stimulus
¶ is an assimulative coefficient

If the response is in terms of concentration and the external stimulus is the load of a material to the water body, we can write:

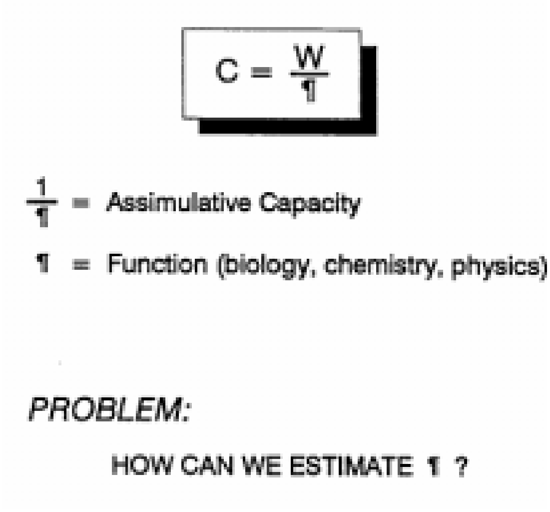
$$\boxed{C = \frac{W}{\P}}$$

NOW

1) if we knew W and ¶ , we could predict the concentration

2) if we set some standard, C_{STD} , and knew ¶ , we could determine how much load we could add and still achieve our standard

3) if we knew C and ¶ , we could back calculate the load required to get to that concentration



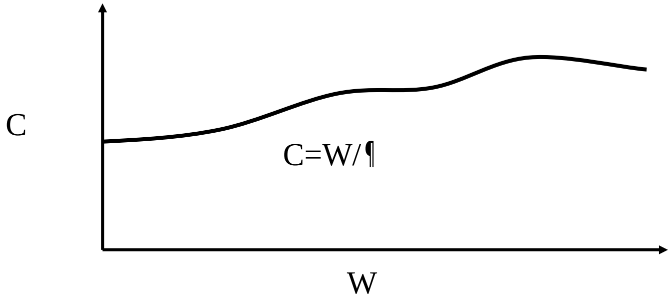
$$\boxed{C = \frac{W}{\P}}$$

$\frac{1}{\P}$ = Assimulative Capacity

¶ = Function (biology, chemistry, physics)

PROBLEM:

HOW CAN WE ESTIMATE ¶ ?

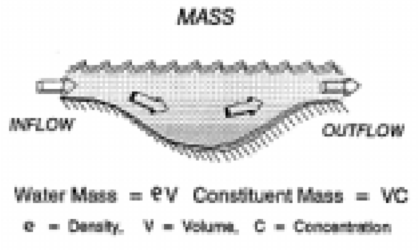


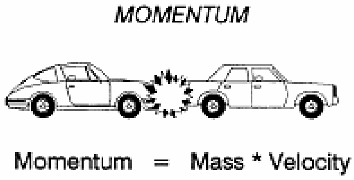
Empirical approach: assume that ¶ is known or related to some external variable and will not be affected by allocation (will not change). Example: determine empirical relationship between DO and waste load based upon measurements

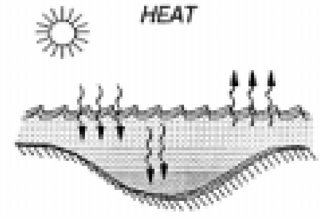
Mechanistic approach: attempt to determine underlying mechanisms affecting ¶ and include those in predictions Example: include processes such as BOD decay, reaeration, etc. in equations relating W and C.

Basic Principal of Mechanistic Models

- **Laws of Conservation**
  - **Conservative properties are those that are not gained or lost through ordinary reactions. Therefore we can account for any change by simply keeping track of all those processes that can cause change**
- **Examples of conservative properties**
    - **Mass (water mass, constituent mass)**
    - **Momentum**
    - **Heat**







BALANCE EQUATION

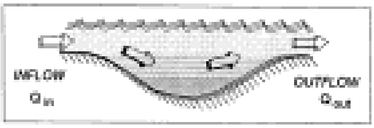
Accumulation = Sources - Sinks

if Sources > Sinks
Accumulation is positive and the material increases.

if Sources < Sinks
Accumulation is negative and the material decreases.

if Sources = Sinks
Accumulation is zero and the quantity of the material does not change.

WATER BALANCE FOR A SIMPLE POND
(Non-Reactive Material)



Water Mass = ρV

ρ [$M L^{-3}$]
V [L^3]

$$\text{Accumulation} = \frac{\text{Change in Water Mass}}{\text{Time}}$$

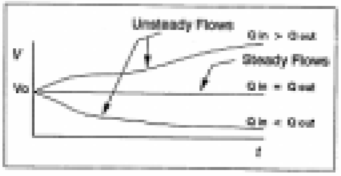
$$= \frac{\Delta \rho V}{\Delta t} \quad \text{Where } \Delta \text{ is Change}$$

$$= \frac{d\rho V}{dt} \quad \text{if } \Delta \text{ is "small"} \quad \left[\frac{M L^3}{L^3 T}\right]$$

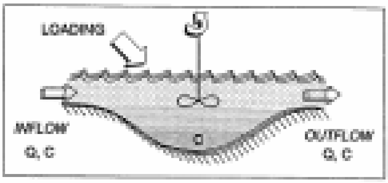
Accumulation = INFLOW - OUTFLOW

$$\frac{d\rho V}{dt} = (Q_{in} - Q_{out})\,\rho$$

$$\text{OR,} \quad \frac{dV}{dt} = Q_{in} - Q_{out} \quad \text{for constant } \rho$$



MASS BALANCE FOR A SIMPLE POND
(Non-Reactive Material)



Accumulation = Inflow - Outflow + Loading

$$= \frac{\text{Change in Mass}}{\text{time}}$$

$$= \frac{\Delta M}{\Delta t} \quad \text{if } \Delta = \text{Change}$$

Mass = Volume * Concentration = VC

if Volume is constant,

$$\text{Accumulation} = V\frac{\Delta C}{\Delta t} \xrightarrow[\text{as } \Delta t \to 0]{} V\frac{dC}{dt}$$

Units $\left[L^3\left(\frac{M}{L^3 T}\right)\right]$

INFLOW = $Q_{in}C_{in}$

OUTFLOW = $Q_{out}C$

LOADING = $W = Q_W C_W$

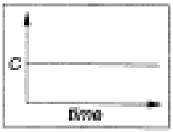
$$\left.\begin{matrix} \\ \\ \\ \end{matrix}\right\} \left[\frac{L^3}{T}\frac{M}{L^3}\right] = \left[\frac{M}{T}\right]$$

$$V\frac{dC}{dt} = Q_{in}C_{in} - Q_{out}C + W$$

SOLUTIONS

1) Steady - State

$$V\overset{\rightarrow 0}{\frac{dC}{dt}} = Q_{in}C_{in} - Q_{out}C + W$$



$$C = \frac{W + Q_{in}C_{in}}{Q_{out}}$$

$$Q_{in} = Q_{out}$$

$$\text{let } W^1 = W + Q_{in}C_{in}$$

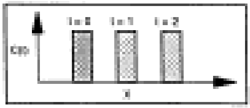
$$C = \frac{W^1}{Q}$$

Therefore, the Assimilative Capacity $1 = \frac{1}{Q}$

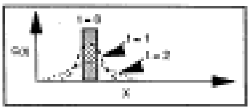
Physical Processes

- Transport = Advection+ Diffusion (or Dispersion)

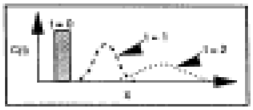
1) Due to advection: organized flow



2) Due to diffusion or diffusion-like processes which tend to reduce gradients



3) Due to advection and diffusion

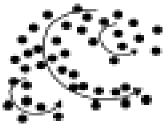


Mixing Processes

MOLECULAR DIFFUSION

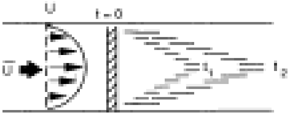
Due to random molecular motion.

TURBULENT DIFFUSION



Due to random turbulent eddie.

DISPERSION



Due to systematic non-uniformatives in velocity distribution.

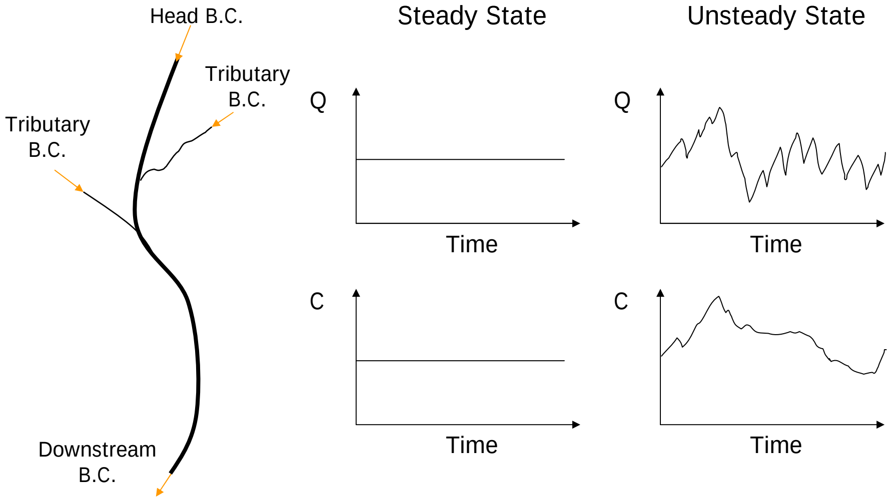
Time

- Steady-state
- Steady-input
- Quasi-dynamic
- Dynamic

Space

- Zero-dimensional (CSTR)
- One-dimensional (x or z)
- Two-dimensional (x-y or x-z)
- Three-dimensional

Definition of Steady and Unsteady State Model



Descriptions of Steady State Model

Background

- Water Quality Model for River Water Quality
  - Steady State (Qual2E-Plus)
  - Unsteady State (Koriv1-Win)
- Assumed Lateral, and Vertical Mixing is completed
- Simulating 15 Water Quality Constituents
- Multiple Discharge, Withdrawal, Tributaries, Inflow and outflow
- Developed from QUAL-I, DOS Environment
- Improved as Qual2E-Plus under Windows Environment

Qual2E-Plus

- Easy Input & Output Data Manipulation
- Developed under .Net Framework Environment
- Channel Shape, Computational Element, Output Results are Shown Graphically
- Allows Comparison of Water Quality Constituents
- Existing as Integrated and Independent Type
- Includes Basic Qual2E Features
- Graphical and Tabulated Output Results

Governing Equation

1D Advection & Diffusion

$$V\frac{\partial c}{\partial t} = \frac{\partial\left(A_c E \frac{\partial c}{\partial x}\right)}{\partial x}dx - \frac{\partial(A_c U c)}{\partial x}dx + V\frac{dc}{dt} + s$$

Acc. **Dispersion** **Advection** **Kinetics** **S/Sink**

Transport

Where, $V =$ Vol, $c =$ Concentration
$A_c =$ Cross section Area
$E =$ Longitudinal Dispersion, $x =$Distance
$U =$ Averaged Velocity
$s =$ Sources(+)/sink (-)

Kinetics

- Carbonaceous BOD (CBOD) and DO

$$\frac{dL}{dt} = -K_1 L - K_3 L$$

and

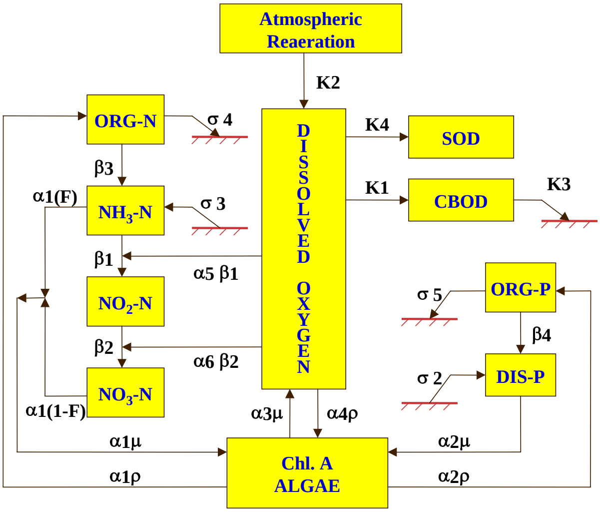
$$\frac{do}{dt} = -K_2(o_S - o) - K_1 L - \frac{K_4}{L}$$

Where,

$L =$ CBOD (mg/l), $o =$ DO (mg/l)
$K_1 =$ BOD decay (d^{-1}), $K_2 =$ reaeration (d^{-1})
$K_3 =$ BOD settling (d^{-1}), $o_S =$ saturated DO (mg/l)
$K_4 =$ Sediment Oxygen Demand (mg^{-2}d^{-1})

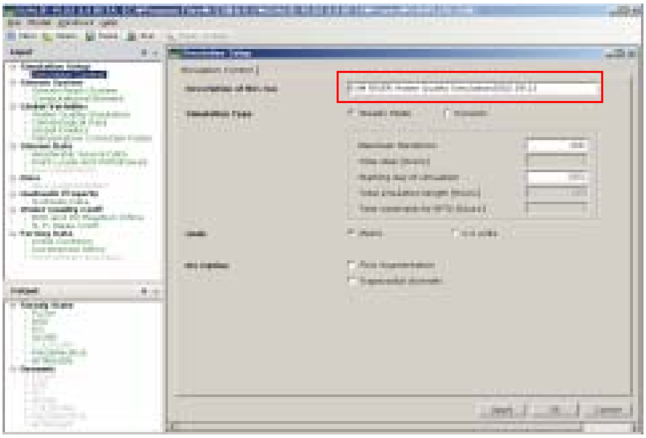
- Reaction Rate K is Temperature related

Qual2E-Plus Kinetics

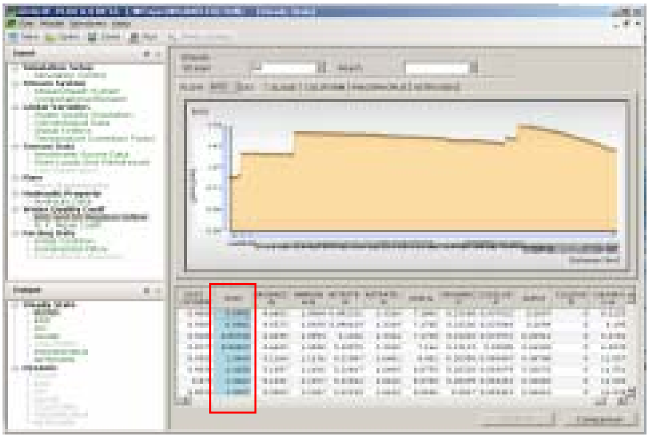


Qual2E-Plus

Simulation Control



Simulation Result of BOD



Further Development

- TMDL Support Tool
- Scenario Comparison Feature
- Future Water Quality Prediction
- Automatic Coefficient Determination Using HEC-RAS
- Observed data Plotting for Parameter Optimization
- Incorporate Optimization algorithm to Determine Reaction Parameters

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Thank You