

CEE 577: Surface Water Quality Modeling

Lecture #23
Thermal Pollution & Modeling
Qual2E: Numerical Solution
(Chapra, L26, L30)

Thermal Pollution

- Concerns
 - direct lethal effects on sensitive plants or animals
 - indirect effects on aquatic ecosystems through effects on the kinetics of biological, physical or chemical processes
- Principal Sources
 - Point sources
 - electric power generating stations (Major)
 - municipal & industrial WWTP's (minor)
 - Non-point Sources
 - long wave atmospheric radiation (H_a)
 - Short wave solar radiation (H_s)

Temperature or Heat Modeling

- Mass Balance is written based on thermal energy

Each term is in:
BTU/m³/d

$$\frac{\partial c}{\partial t} = -\frac{1}{A} \frac{\partial(Qc)}{\partial x} + E \frac{\partial^2 c}{\partial x^2} + kc + \frac{H_N}{z}$$

Areal source/sink
(BTU/m²/d)

zero

- and we relate this to temperature by: $c = \rho c_H (T - T_0)$
 - where: c = heat concentration or energy (BTU/m³)
 - ρ = density of water (g/m³)
 - C_H = heat capacity of water (BTU/g/°C)
 - T_0 = arbitrary “frame of reference” temperature (°C)

- Substituting in we get:

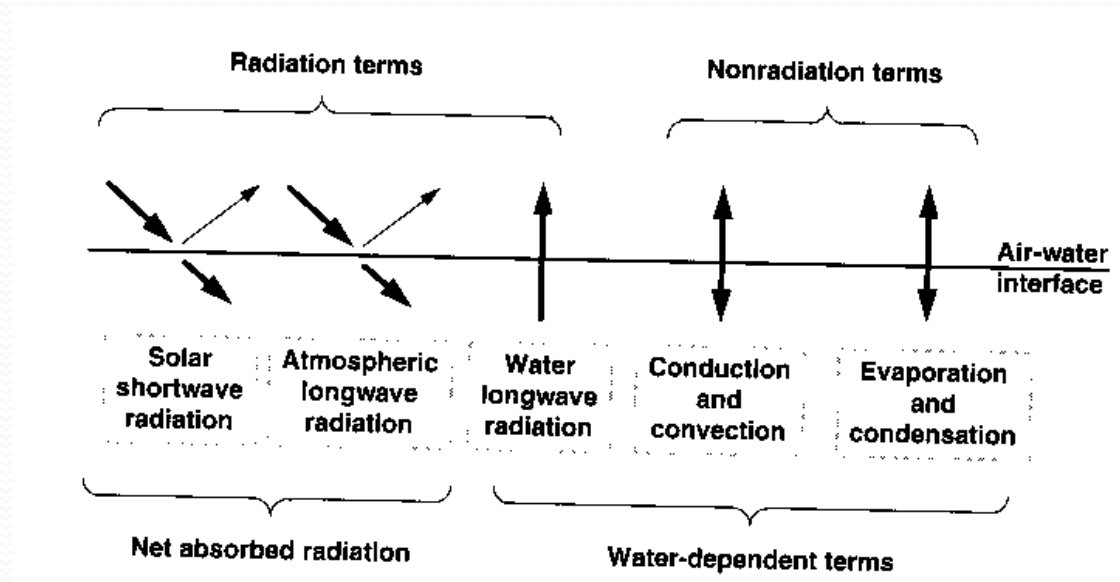
$$\frac{\partial T}{\partial t} = -\frac{1}{A} \frac{\partial(QT)}{\partial x} + E \frac{\partial^2 T}{\partial x^2} + \frac{H_N}{\rho c_H z}$$

Heat Modeling (cont.)

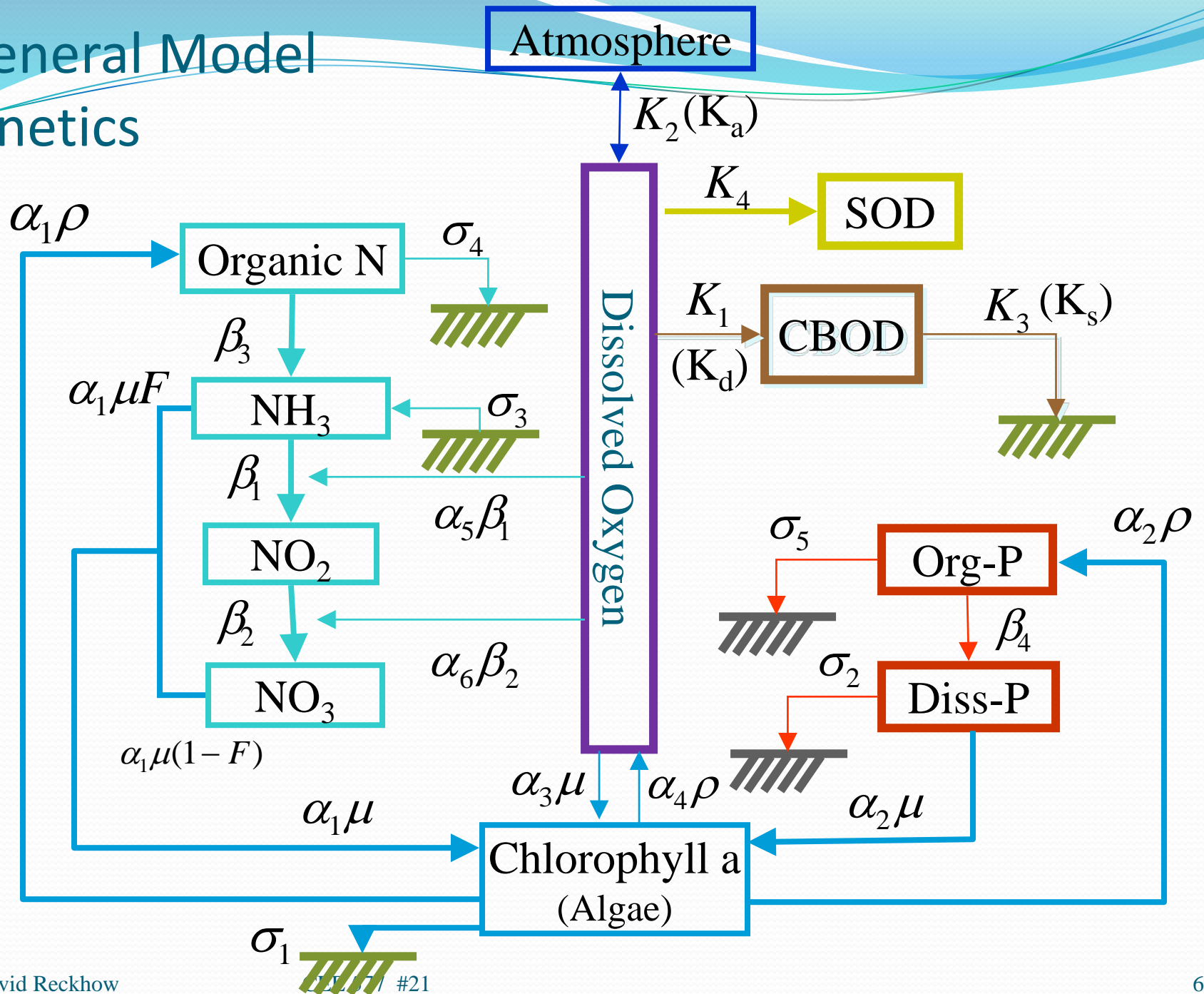
- Determination of H_N
 - Refer to:
 - Computer Program Documentation for the Enhanced Stream Water Quality Model QUAL2E, USEPA publication #EPA/600/3-85/065, August 1985.
 - QUAL2K: A Modeling Framework for Simulating River and Stream Water Quality, Chapra et al., 2008
 - Also some treatment in Chapra
 - (Lecture 30)

Total Surface Heat Flux

- Chapra
 - Fig 30.3



General Model Kinetics

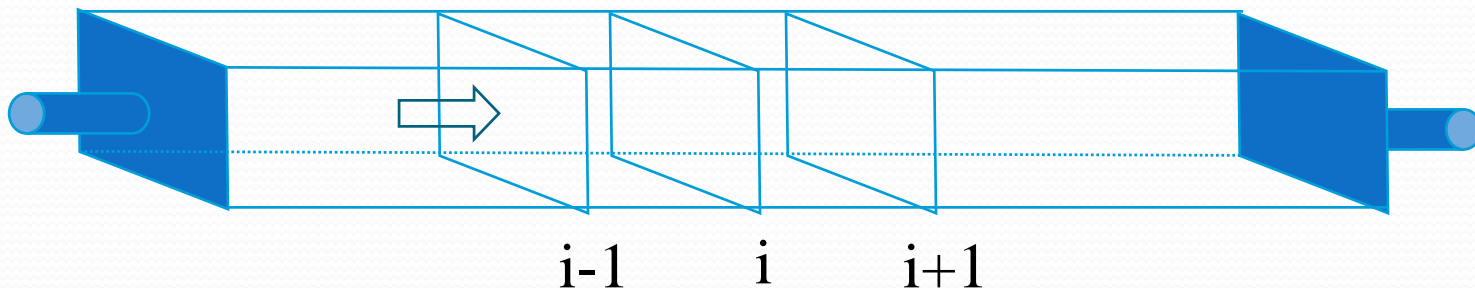


Numerical Solutions (QUAL2E)

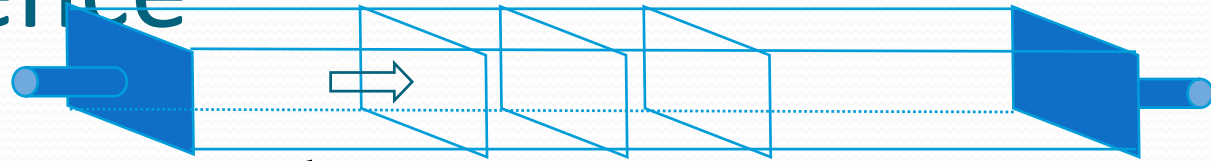
- The problem
 - need to develop numerical estimates for the first and second derivatives of concentration versus distance

$$\frac{\partial c}{\partial t} = -U \left(\frac{\partial c}{\partial x} \right) + E \left(\frac{\partial^2 c}{\partial x^2} \right)$$

- The solution
 - Finite Difference



Finite Difference



- Euler-Cauchy Approach

- Forward Difference

$$\left. \frac{\partial c}{\partial x} \right|_i \approx \frac{c_{i+1} - c_i}{\Delta x}$$

- Backward Difference

$$\left. \frac{\partial c}{\partial x} \right|_i \approx \frac{c_i - c_{i-1}}{\Delta x}$$

- Central or Centered Difference

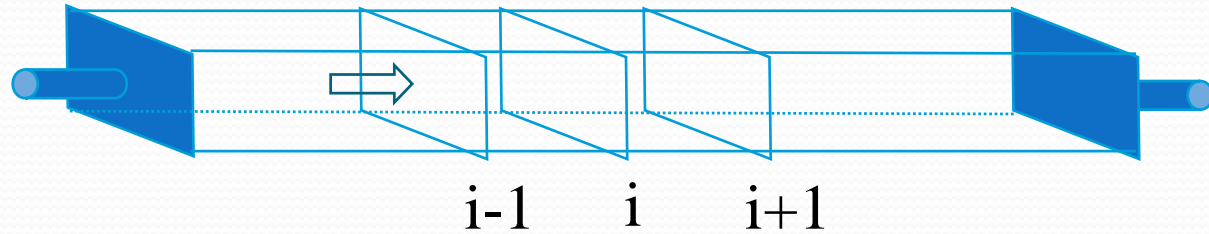
$$\left. \frac{\partial c}{\partial x} \right|_i \approx \frac{c_{i+1} - c_{i-1}}{2\Delta x}$$

First
Order
Accurate

Second
Order
Accurate

But less stable

Finite Difference (cont.)



- Formulation:
Explicit

- backward difference
- forward difference
- Gives centered difference

$$\begin{aligned}\frac{\partial^2 c}{\partial x^2} \Big|_i &\approx \frac{\frac{\partial c}{\partial x} \Big|_i - \frac{\partial c}{\partial x} \Big|_{i-1}}{\Delta x} \\ &\approx \frac{(c_{i+1} - c_i) / \Delta x - (c_i - c_{i-1}) / \Delta x}{\Delta x} \\ &\approx \frac{c_{i+1} - 2c_i + c_{i-1}}{\Delta x^2}\end{aligned}$$

The Explicit Approach

- The differential equation:

$$\frac{\partial c}{\partial t} = -U \frac{\partial c}{\partial x} + E \frac{\partial^2 c}{\partial x^2}$$

- Becomes:

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} = -U \frac{c_{i+1}^n - c_{i-1}^n}{2\Delta x} + E \frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{\Delta x^2}$$

- And rearranging:

$$c_i^{n+1} = c_i^n + \left(-U \frac{c_{i+1}^n - c_{i-1}^n}{2\Delta x} + E \frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{\Delta x^2} \right) \Delta t$$

The QUAL2E approach

- Classical Implicit Backwards Difference

$$C_i^{n+1} = C_i^n + \left(-U \frac{C_i^{n+1} - C_{i-1}^{n+1}}{\Delta x} + E \frac{C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1}}{\Delta x^2} + kC_i^{n+1} + z_i \right) \Delta t$$

- k is the rate constant for all internal processes and reactions (e.g., biodegradation)
- z_i is the sum of all internal sources and sinks
 - e.g., SOD
- Solved using matrix subroutines

- To next lecture