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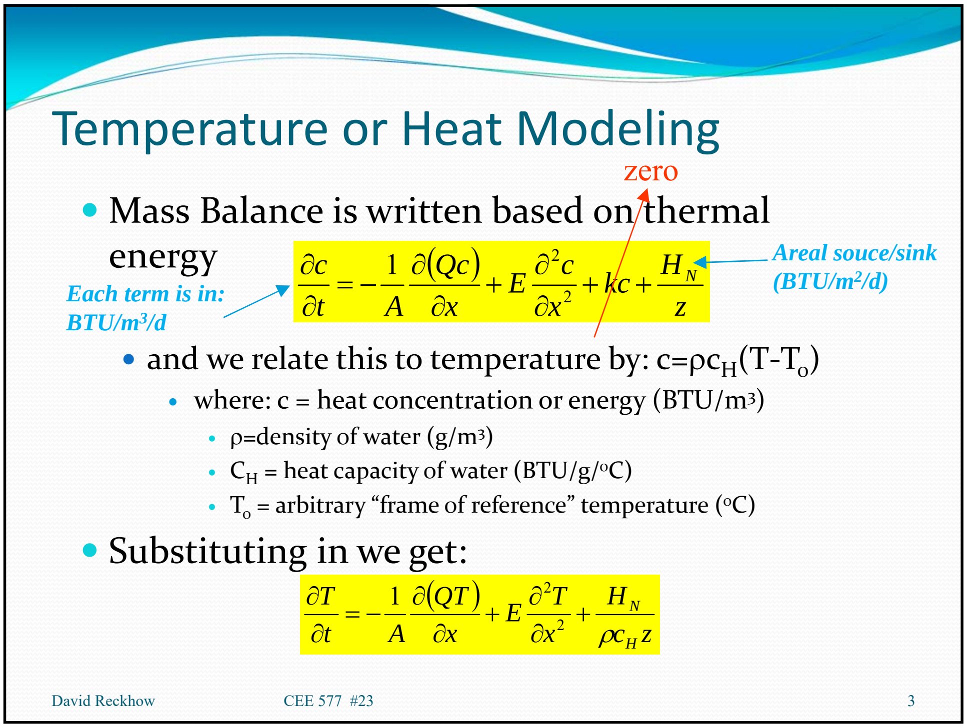
CEE 577: Surface Water Quality Modeling

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

zero

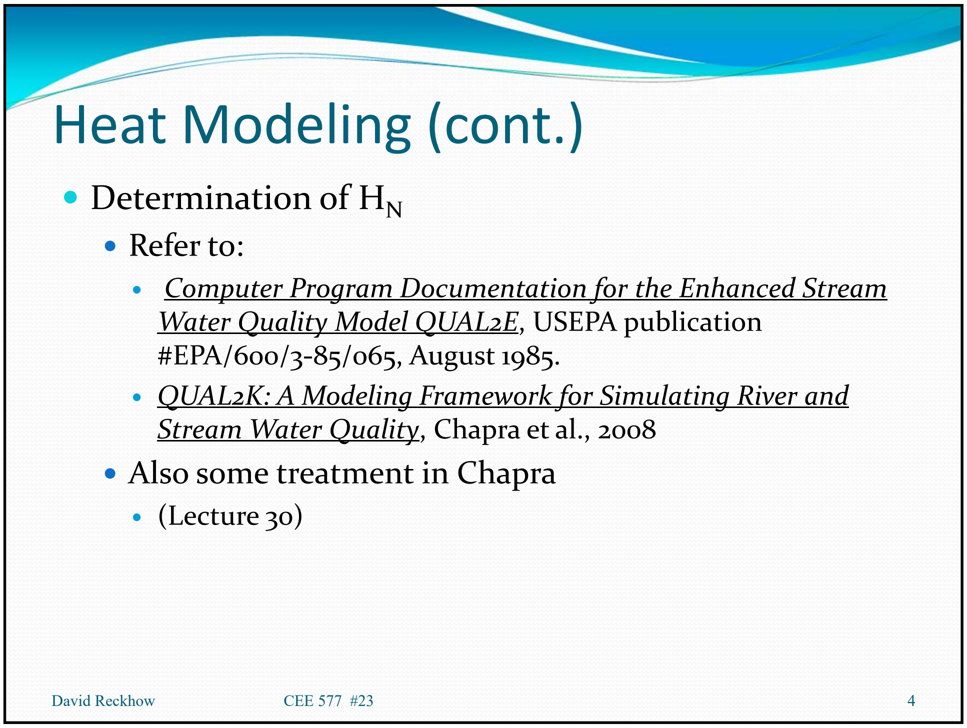
Each term is in: BTU/m³/d

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

Areal souce/sink (BTU/m²/d)

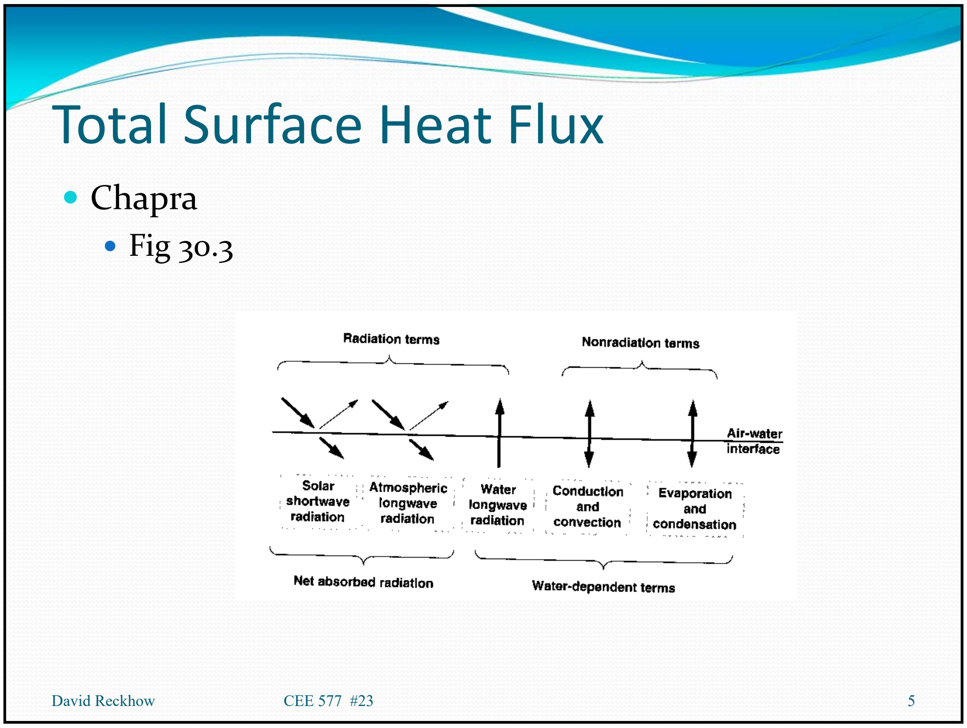
  - and we relate this to temperature by: $c = \rho c_H (T - T_o)$
    - where: c = heat concentration or energy (BTU/m³)
      - ρ=density of water (g/m³)
      - C_H = heat capacity of water (BTU/g/°C)
      - T_o = arbitrary "frame of reference" temperature (°C)
- Substituting in we get:

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



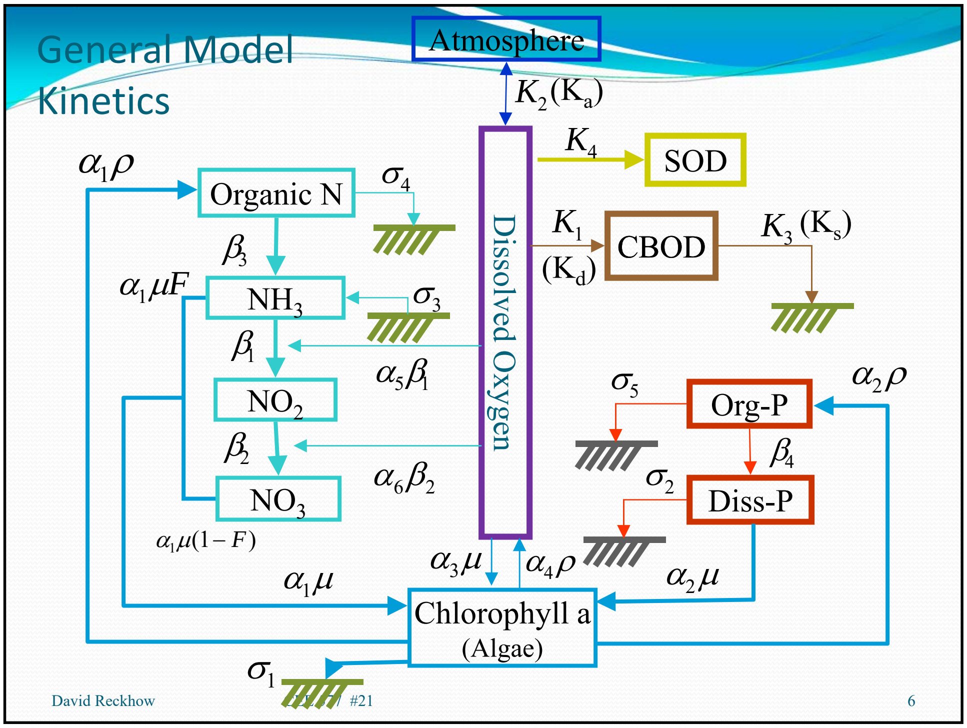
Heat Modeling (cont.)

- 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)

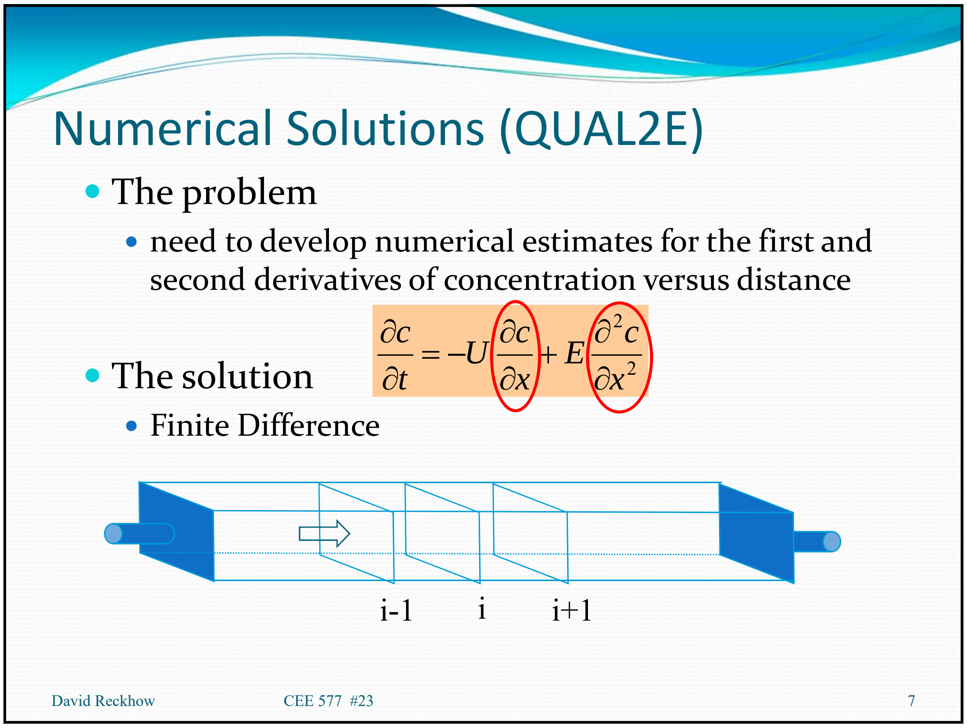


Total Surface Heat Flux

- Chapra
  - Fig 30.3



General Model Kinetics

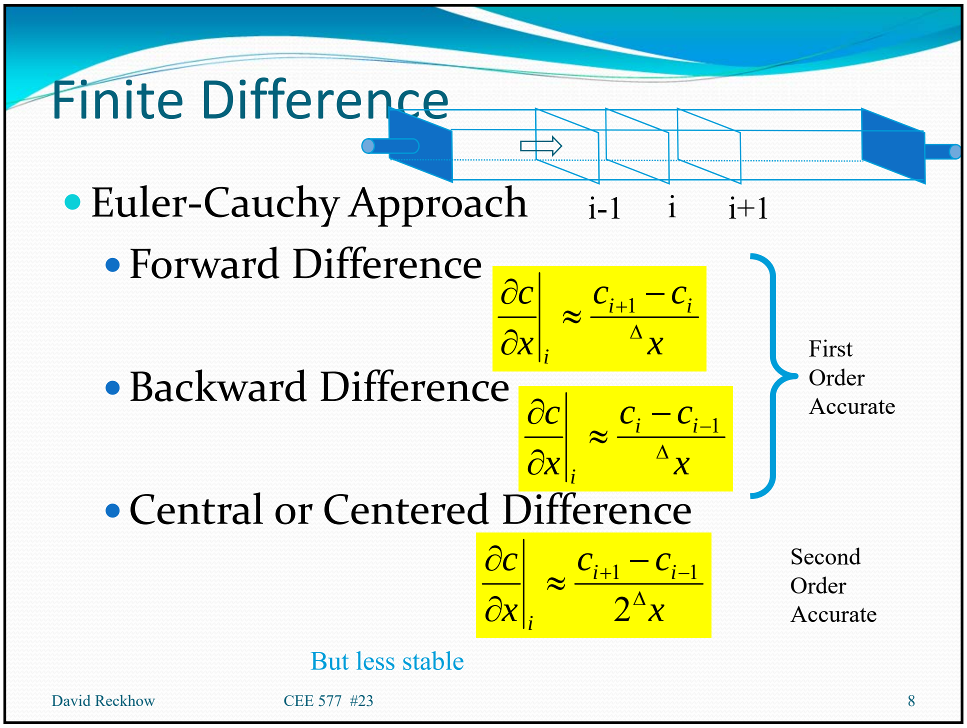


Numerical Solutions (QUAL2E)

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

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

i-1 i i+1



Finite Difference

i-1 i i+1

- Euler-Cauchy Approach
  - Forward Difference

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

  - Backward Difference

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

First Order Accurate

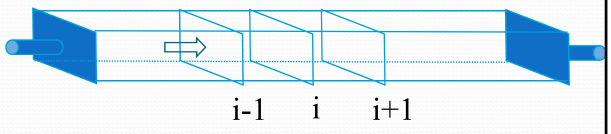
  - Central or Centered Difference

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

Second Order Accurate

But less stable

Finite Difference (cont.)



- Formulation: Explicit
  - backward difference
  - forward difference
  - Gives centered difference

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

$$\approx \frac{(c_{i+1}-c_i)/\Delta x - (c_i-c_{i-1})/\Delta x}{\Delta x}$$

$$\approx \frac{c_{i+1}-2c_i+c_{i-1}}{\Delta x^2}$$

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