Computational Hydraulics

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Contaminant Transport in Open Channels and Pipes

Module 11

5 lectures

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Contaminant transport

- Contaminant transport modeling studies are usually concerned with the movement within an aquifer system of a solute.
- These studies have become increasingly important with the current interest on water pollution.
- Heat transport models are usually focused on developing geothermal energy resources.
- Pollutant transport is an obvious concern relative to water quality management and the development of water protection programs

Definition of terms

Terminologies related to contaminant transport

- ***Diffusion**: It refers to random scattering of particles in a flow to turbulent motion*
- ***Dispersion**: This is the scattering of particles by combined effect of shear and transverse diffusion*
- ***Advection**: The advective transport system is transport by the imposed velocity system*

Introduction to ADE equation

- The one dimensional formulation of conservative tracer mass balance for advective-dispersive transport process is

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D_l \frac{\partial^2 C}{\partial x^2} \pm R$$

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$u\frac{\partial C}{\partial x}$ = advection of tracer with fluid

$D_l \frac{\partial^2 C}{\partial x^2}$ = molecular diffusion +Hydrodynamic dispersion

$\frac{\partial C}{\partial t}$ = time rate of change of concentration at a point

R = reaction term depends on reaction rate and concentration (chemical or biological, not considered in the present study)

Few simple solutions

- Bear discussed several analytical solutions to relatively simple, one-dimensional solute transport problems. However, even simple solutions tend to get overwhelmed with advanced mathematics.

- As an example, consider the one-dimensional flow of a solute through the soil column, the boundary conditions represented by the step function input are described mathematically as:

$$C(1,0) = 0 \qquad 1 \geq 0$$

$$C(0,t) = C_0 \qquad t \geq 0$$

$$C(\infty,t) = 0 \qquad t \geq 0$$

Few simple solutions

- For these boundary conditions the solution to ADE equation for a saturated homogeneous porous medium is:

$$\frac{C}{C_o} = \frac{1}{2}\left[erfc\frac{(1-\bar{v}t)}{2\sqrt{D_l t}} + \exp\left(\frac{\bar{v}_l}{D_l}\right) erfc\left(\frac{1+\bar{v}t}{2\sqrt{D_l t}}\right)\right]$$

- *erfc* represents the complimentary error function; l is the distance along the flow path; and v is the average water velocity.
- For conditions in which the dispersivity D_l of the porous medium is large or when 1 or t is large, the second term on the right-hand side of equation is negligible.

Few simple solutions

- This equation can be used to compute the shapes of the breakthrough curves and concentration profiles
- Analytical models represent an attractive alternative to both physical and numerical models in terms of decreased complexity and input data requirements.
- Analytical models are often only feasible when based on significant simplifying assumptions, and these assumptions may not allow the model to accurately reflect the conditions of interest.
- Additionally, even the simplest analytical models tend to involve complex mathematics

Solution of ADE through FD methods

Using implicit finite central difference method

$$\frac{\left(D_l \frac{\partial C}{\partial x}\right)_{i+\frac{1}{2}} - \left(D_l \frac{\partial C}{\partial x}\right)_{i-\frac{1}{2}}}{\Delta x} - u_i \frac{C_{i+1} - C_i}{\Delta x} = \frac{C_i - C_0}{\Delta t}$$

$$(D_l)_{i+\frac{1}{2}} \frac{C_{i+1} - C_i}{\Delta x^2} - (D_l)_{i-\frac{1}{2}} \frac{C_i - C_{i-1}}{\Delta x^2} - u_i \frac{C_{i+1} - C_i}{\Delta x} = \frac{C_i - C_0}{\Delta t}$$

$$\frac{(D_l)_{i-\frac{1}{2}}}{\Delta x^2} C_{i-1} - \left(\frac{(D_l)_{i-\frac{1}{2}}}{\Delta x^2} + \frac{(D_l)_{i+\frac{1}{2}}}{\Delta x^2} - \frac{u_i}{\Delta x} + \frac{1}{\Delta t} \right) C_i + \left(\frac{(D_l)_{i+\frac{1}{2}}}{\Delta x^2} - \frac{u_i}{\Delta x} \right) C_{i+1} = -\frac{C_0}{\Delta t}$$

Solution of ADE through FD methods

Continued...

$$-\frac{(D_l)_{i-\frac{1}{2}}}{\Delta x^2}C_{i-1}+\left(\frac{(D_l)_{i-\frac{1}{2}}}{\Delta x^2}+\frac{(D_l)_{i+\frac{1}{2}}}{\Delta x^2}-\frac{u_i}{\Delta x}+\frac{1}{\Delta t}\right)C_i-\left(\frac{(D_l)_{i+\frac{1}{2}}}{\Delta x^2}-\frac{u_i}{\Delta x}\right)C_{i+1}=\frac{C_0}{\Delta t}$$

- The above equation can be written in matrix form as:

1. For internal nodes

$$AAC_{i-1}+BBC_i+CCC_{i+1}=DD$$

Solution of ADE through FD methods

2. For Right boundary condition:

Using forward finite difference formation in the right boundary, flux can be written as follows as

$$\frac{C_{i+1} - C_i}{\Delta x} = flux$$

$$C_{i+1} = C_i + flux(\Delta x)$$

$$AAC_{i-1} + BBC_i + CC(C_i + flux(\Delta x)) = DD$$

$$AAC_{i-1} + (BB + CC)C_i = DD - CCflux(\Delta x)$$

Solution of ADE through FD methods

3. For Left boundary condition:

- At the left boundary, initial condition and Dirichlet condition are used which is given below:

$$C(x,0) = C_i \qquad x > 0;$$

$$C(0,t) = C_0 \qquad t > 0;$$

- Using backward finite difference formation in the right boundary, flux can be written as follows

$$\frac{C_i - C_{i-1}}{\Delta x} = flux$$

Solution of ADE through FD methods

Continued $$C_{i-1} = C_i - flux(\Delta x)$$

$$(AA + BB)C_i + CCC_{i+1} = DD + AA(flux\Delta x)$$

The above three equations are solved for C_i at all the nodes for the mesh. Thomas Algorithm can be used to solve the set of equations.

Problems linked with solution methods

- The contaminant transport in open channels and pipes are solved through various computer models.
- Because of their increased popularity and wide availability, it is necessary to note the limitations of these models
- The first limitation is the requirement of significant data
- Some available data may not be useful
- The second limitation associated with computer models is their required boundary conditions

Problems linked with solution methods

- Computer models can be very precise in their predictions, but these predictions are not always accurate
- The accuracy of the model depends on the accuracy of the input data
- Some models may exhibit difficulty in handling areas of dynamic flow such as they occur very near wells
- Another problem associated with some computer models is that they can be quite complicated from a mathematical perspective

Problems linked with solution methods

- These computer modeling are also time consuming
- This is usually found to be true if sufficient data is not available
- Uncertainty relative to the model assumption and usability must be recognized
- The computer model has been some time misused, as for example the model has been applied to the cases where it is not even applicable.

Demonstration of methods for open channel flows

- Mass transport in streams or long open channels is typically described by a one-dimensional
- Advection {dispersion equation, in which the longitudinal dispersion co-efficient is the combination of various section-averaged hydrodynamic mixing effects.
- The classical work of Taylor (1953, 1954) established the fact that the primary cause of dispersion in shear flow is the combined action of lateral diffusion and differential longitudinal advection.

Demonstration of methods for open channel flows

- The transport of solutes in streams is affected by a suite of physical, chemical and biological processes, with the relative importance of each depending on the geo-environmental setting and properties of the solutes.
- For many species, chemical and biological reactions are just as influential as the physical processes of advection and dispersion in controlling their movement in an aquatic system like a stream.

Demonstration of methods for open channel flows

- Though chemical reactions and phase exchange mechanisms have now been incorporated into some applied transport models.

- Theoretical studies into these chemical effects on the physical transport have been very limited.

- There lacks, for example, a systematic understanding of the effects of sorption kinetics on the longitudinal dispersion: dispersion is conventionally considered to be affected by physical and hydrodynamic processes only.

Demonstration of methods for pipe flows

- An important component of a water supply systems is the distribution system which conveys water to the consumer from the sources.
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- Drinking water transported through such distribution systems can undergo a variety of water quality changes in terms of physical, chemical, and biological degradation.
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- Water quality variation during transportation in distribution systems may be attributed to two main aspects of reasons. One is internal degradation, and the other is external intrusion.

Demonstration of methods for pipe flows

- The internal factors including physical, chemical, and biological reaction with pipe wall material that degrades water quality.
- Furthermore, recent evidence has demonstrated that external contaminant intrusion into water distribution systems may be more frequent and of a great importance than previously suspected.
- In conventional (continuous) water distribution systems, contaminant may enter into water supply pipe through cracks where low or negative pressure occurs due to transient event.

Demonstration of methods for pipe flows

- The sources of contaminant intrusion into water distribution systems are many and various. But leaky sewer pipes, faecal water bodies, and polluted canals may be the primary sources for water distribution systems contamination.

- Both continuous and intermittent water distribution systems might suffer from the contaminant intrusion problem, and the intermittent systems were found more vulnerable of contaminant intrusion.

Demonstration of methods for pipe flows

- Chlorination in pipe flow is required to control the biological growth, which on the other hand results in water quality deterioration.

- Pipe condition assessment component simulates contaminant ingress potential of water pipe.

- Contaminant seepage will be the major component of the model. Its objective will be to simulate the flow and transport of contaminant in the soil from leaky sewers and other pollution sources to water distribution pipes.

Demonstration of methods for pipe flows

- The equations to be applied to simulate contaminant flow through the pipes are similar to open channel contaminant transport.
- The process involved during the contaminants transport includes advection, dispersion and reaction, etc., which results in varying concentration of the contaminants during its transportation.

Assignments

1. Considering the one-dimensional flow of a solute through the soil column, write a computer program for solving the given contaminant transport equation by finite difference technique. The boundary conditions represented by the step function input are described mathematically as:

$$C(1,0) = 0 \qquad 1 \geq 0$$

$$C(0,t) = C_0 \qquad t \geq 0$$

$$C(\infty,t) = 0 \qquad t \geq 0$$

   Compare and discuss the results with the analytical method.

2. Write the governing equation for transport of contaminant in a pipe, neglecting advection and dispersion terms, and solve to get analytical solution of the same.