Presentation 7

MT3DMS—Solution Schemes

MT3DMS User Manual


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MT3DMS: A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems; Documentation and User's Guide

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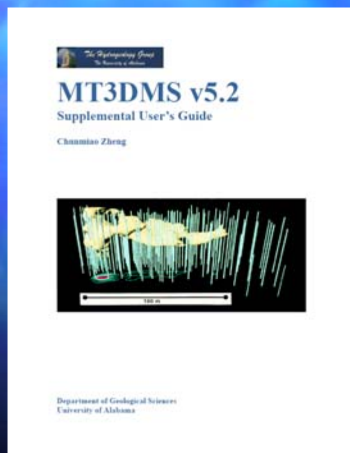
http://hydro.geo.ua.edu/mt3d/mt3dmanual.pdf

MT3DMS Supplemental Guide


MT3DMS v5.2
Supplemental User's Guide
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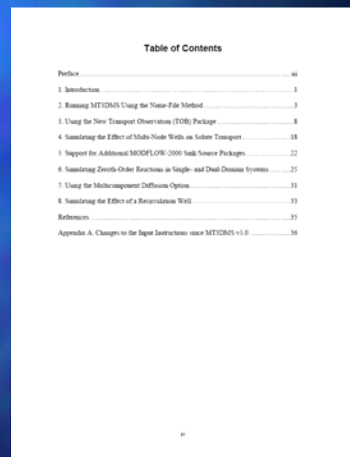
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History of MT3D

SSP&A	USEPA	UA/DoD
Ver.1.04 10/1990	Ver.1.04 10/1990	
Ver.1.10 01/1992	Ver.1.10 01/1992	
Ver.1.80 10/1992		
Ver.1.85 06/1994		DoD_1.5 07/1996
MT3D'96 06/1996		MT3DMS 3.0 05/1998
		MT3DMS 4.0 08/2001
		MT3DMS 5.2 10/2006
		MT3DMS 5.3 2/2010

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Mathematical Model of Solute Transport

- Governing equations
- Initial conditions
- Boundary conditions

Solutions:

- Analytical
- Numerical

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Governing Equations

- Flow equations
  - As solved in MODFLOW

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)+W=S_s\frac{\partial h}{\partial t}$$

  - As solved in SEAWAT

$$\frac{\partial}{\partial x}\left[\rho K_{fx}\left(\frac{\partial h_f}{\partial x}+\frac{\rho-\rho_f}{\rho_f}\frac{\partial z}{\partial x}\right)\right]+\frac{\partial}{\partial y}\left[\rho K_{fy}\left(\frac{\partial h_f}{\partial y}+\frac{\rho-\rho_f}{\rho_f}\frac{\partial z}{\partial y}\right)\right]+\frac{\partial}{\partial z}\left[\rho K_{fz}\left(\frac{\partial h_f}{\partial z}+\frac{\rho-\rho_f}{\rho_f}\right)\right]=\rho S_f\frac{\partial h_f}{\partial t}+\theta\frac{\partial \rho}{\partial C}\frac{\partial C}{\partial t}-\rho_s q_s$$

- Transport equation (as solved in MT3D)

$$\frac{\partial C}{\partial t}=-\nabla\cdot(\vec{v}C)+\nabla\cdot(D\cdot\nabla C)-\frac{q_s}{\theta}C_s+\sum_{k=1}^{N}R_k$$

Governing Equations: Linkage Between Flow and Transport

- Constant density

concentrations are affected by flow

$$v_i = \frac{q_i}{\theta}$$

- Variable density

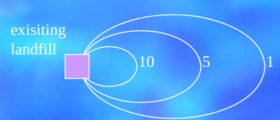
concentrations are affected by flow

$$v_i = \frac{q_i}{\theta}$$

flow is affected by concentrations

$$\rho = \rho_f + \frac{\partial \rho}{\partial C} C$$

Initial Conditions



C(x,y,z,0) determined from field data

(a) Initial condition characterized by an existing plume.

potential waste disposal site

C(x,y,z,0) = 0

(b) Initial condition characterized by zero concentration everywhere.

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Boundary Conditions

- Constant-concentration [Dirichlet]
- Specified concentration gradient (i.e. dispersive flux) [Neumann]
  - *a special case is zero dispersive flux*
- Specified total mass flux (i.e., advective and dispersive) [Cauchy]
  - *a special case is zero mass flux*

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Boundary Conditions in MT3D

- Specified-concentration boundary (try to avoid)
- No flow boundary in MODFLOW is automatically treated as zero mass flux boundary
- All other MODFLOW boundaries (including specified-flow, head-dependent flux, and constant head) are automatically treated as specified mass flux, with mass flux = QC, where Q is specified by user (WEL) or determined by MODFLOW (eg. GHB). Dispersive flux is always assumed to be negligible.

Solution of the Transport Equation

$$\frac{\partial C}{\partial t} = \underbrace{-\nabla \cdot (\vec{v}C)}_{\text{ADV}} + \underbrace{\nabla \cdot (D \cdot \nabla C)}_{\text{DSP}} \underbrace{- \frac{q_s}{\theta} C_s}_{\text{SSM}} + \underbrace{\sum_{k=1}^{N} R_k}_{\text{RCT}}$$

first order second order

- Fundamental difficulty: the need to treat simultaneously the first-order (hyperbolic) advection term and the second-order (parabolic) dispersion term

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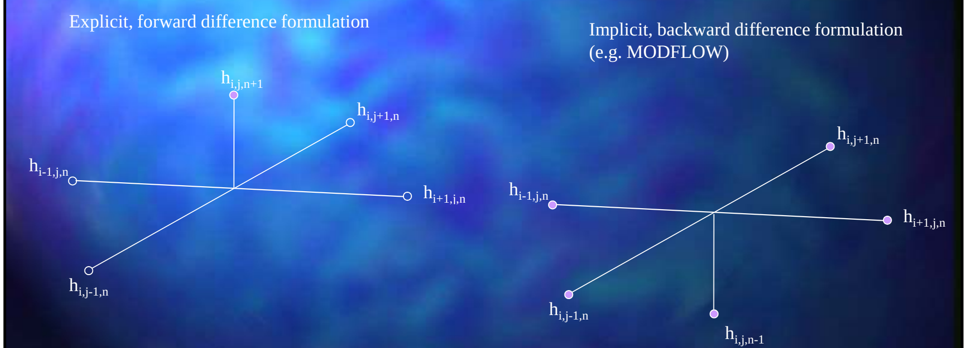
Solution Methods

- Eulerian
  - Fixed grid (standard finite difference or finite element)
- Lagrangian
  - Deforming grid or deforming coordinate in a fixed grid (particle based)
- Mixed Eulerian-Lagrangian
  - Combination of Eulerian and Langrangian methods

Example of Explicit Versus Implicit Methods



Solution Approaches

- Advection term
  - Multiple approaches
- Dispersion, Sink/Source, Chemical Reaction
  - Explicit finite-difference method (original MT3D). Simple but subject to timestep constraints
  - Implicit finite-difference method using GCG solver (MT3DMS). Requires a matrix solver, but no constraint on timestep size

Solution Schemes (advection term)

- Standard finite difference
  - Upstream weighting
  - Central-in-space weighting

- Method of characteristics
- Modified method of characteristics
- Hybrid method of characteristics

- 3rd-order total-variation diminishing (TVD) [ultimate]

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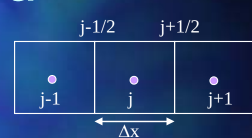
Finite-Difference Method



$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x}$$

$$D\frac{\partial^2 C}{\partial x^2} = D\frac{\left(\frac{\partial C}{\partial x}\right)_{j+1/2} - \left(\frac{\partial C}{\partial x}\right)_{j-1/2}}{\Delta x} = D\frac{C_{j+1} - 2C_j + C_{j-1}}{(\Delta x)^2}$$

$$v\frac{\partial C}{\partial x} = v\frac{C_{j+1/2} - C_{j-1/2}}{\Delta x}$$

Central-in-space

$$C_{j+1/2} = \tfrac{1}{2}\left(C_j + C_{j+1}\right)$$

Upstream (upwind)

$C_{j+1/2} = C_j$ or $C_{j+1/2} = C_{j+1}$

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Advantages and Disadvantages of FDM

- Advantages
  - Mass conservative
  - Computationally efficient for dispersion dominated problems
  - No numerical difficulty for distorted model grids or in the presence of many sinks/sources
- Disadvantages
  - Suffer from numerical dispersion errors for advection-dominated problems or from artificial oscillation
  - To minimize numerical dispersion errors, fine spatial discretization may be necessary, i.e., to satisfy the Peclet number constraint:

$$\frac{v_x \Delta x}{D_{xx}} = \frac{\Delta x}{\alpha_L} \le 2-4$$

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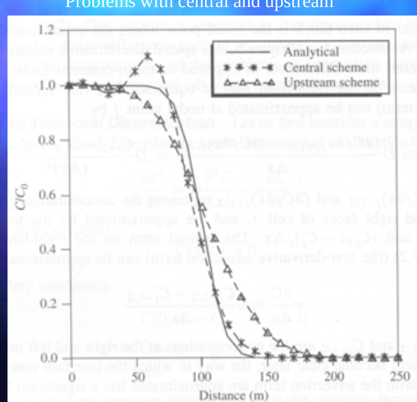
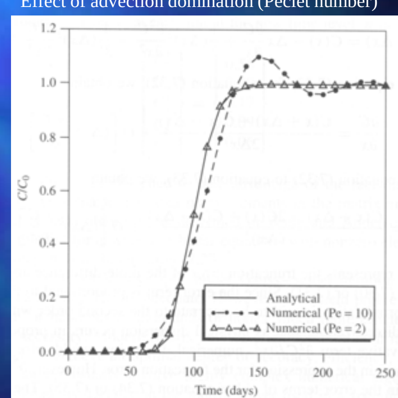
Numerical Problems Associated with FDM

Problems with central and upstream



Effect of advection domination (Peclet number)



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Courant Number

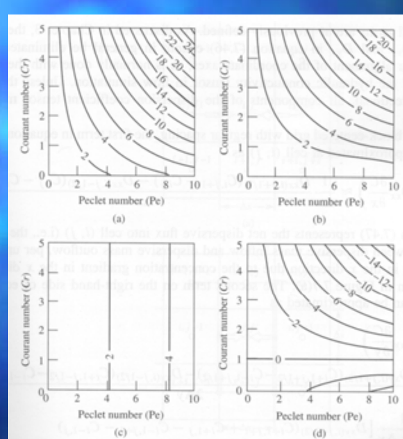
- Number of cells, or fractional cell distance, that a particle is advected in one timestep

$$C_r = \frac{v\Delta t}{\Delta x}$$

Ratio of Numerical to Physical Dispersion

Implicit, upstream

Implicit, central-in-space

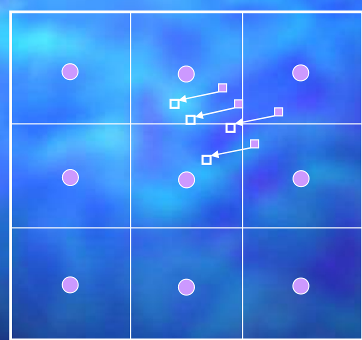


Crank-Nicolson, upstream

Explicit, upstream

For simple, one-dimensional flow (Zheng and Bennett, 2002, p. 189)

Method of Characteristics (MOC)



Each particle carries a volume and a concentration

$$C_m^{n*} = \frac{\sum_{p=1}^{N} C_p^n V_p}{\sum_{p=1}^{N} V_p}$$

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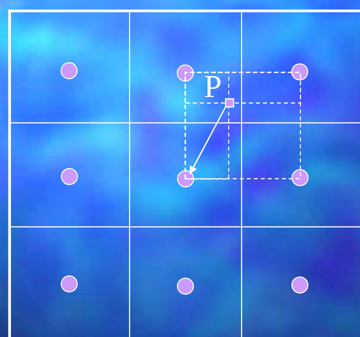
Particle Allocation

- Uniform Approach
  - Particles distributed evenly throughout active model domain
- Dynamic Approach
  - Particles placed only in areas with high concentration gradients

Modified Method of Characteristics (MMOC)



Concentration at point P is interpolated from those at neighboring nodes

$$C_m^{n*} = C^n(P) = C^n(-v\Delta t)$$

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Hybrid Method of Characteristics (HMOC)

- MOC is most effective when advection dominates over dispersion, while MMOC is only suitable when advection is less dominant
- Apply MOC where advection dominates, dynamically adding particles as needed
- Automatically switch to MMOC where advection is less dominant, removing particles that are no longer needed

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Advantages and Limitation of Particle Methods

- Advantages
  - Virtually eliminate numerical dispersion
  - Computationally efficient for highly advection-dominated problems
- Disadvantages
  - May have mass balance discrepancy problems, particularly when model grid is highly irregular
  - Calculated concentration breakthrough curves may be “rough”
  - Computer memory intensive, particularly for multi-species simulations, with a set of particles for each species

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Third-Order TVD (ULTIMATE)

- Also referred to as higher-order finite-difference or finite-volume method.
- TVD—Total Variation Diminishing
  - The sum of concentration differences between adjacent nodes diminishes over successive transport steps
- ULTIMATE—Universal Limiter for Transient Interpolation Modeling of the Advective Transport Equations

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TVD Concept

- Use third-order polynomial (biased in the upstream direction) to interpolate concentration at $-v\Delta t$
- Employ flux limiter to adjust interface concentrations if conditions indicate spurious oscillations could be a problem
- Described in MT3DMS Manual (Zheng and Wang, 1998)

Advantages and Disadvantages of TVD

- Advantages
  - Mass conservative
  - Minimal numerical dispersion and artificial oscillation for advection dominated problems
  - No numerical difficulty for distorted model grids or in the presence of many sinks/sources
- Disadvantages
  - Could be computationally demanding
  - May not be as effective as MOC in eliminating numerical dispersion for purely advective problems

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Generalized Conjugate Gradient (GCG) Solver

- General purpose iterative solver
- Three preconditioning options
  - Jacobi
  - Symmetric Successive Over Relaxation
  - Modified Incomplete Cholesky (MIC) *(fewer iterations, more memory)*
- Lanczos/ORTHOMIN acceleration scheme
- Two iteration loops (outer loop only required if matrix coefficients are a function of concentration: non-linear sorption)

List of Solution Options in MT3D

Group	Solution Options for Advection	Solution Options for Dispersion, Sinks/Source and Reaction
A	Particle Tracking Based Eulerian-Lagrangian Methods ▪MOC ▪MMOC ▪HMOC	Explicit Finite Difference
B	Particle Tracking Based Eulerian-Lagrangian Methods ▪MOC ▪MMOC ▪HMOC	Implicit Finite Difference
C	Explicit Finite Difference ▪Upstream weighting	Explicit Finite Difference
D	Implicit Finite Difference Upstream weighting Central-in-space weighting	Implicit Finite Difference
E	Explicit Third-Order TVD	Explicit Finite Difference
F	Explicit Third-Order TVD	Implicit Finite Difference

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