MT3DMS

Modular 3-D Transport model
MS denotes the Multi-Species structure for accommodating add-on reaction packages

Downloads & a wealth of information at:

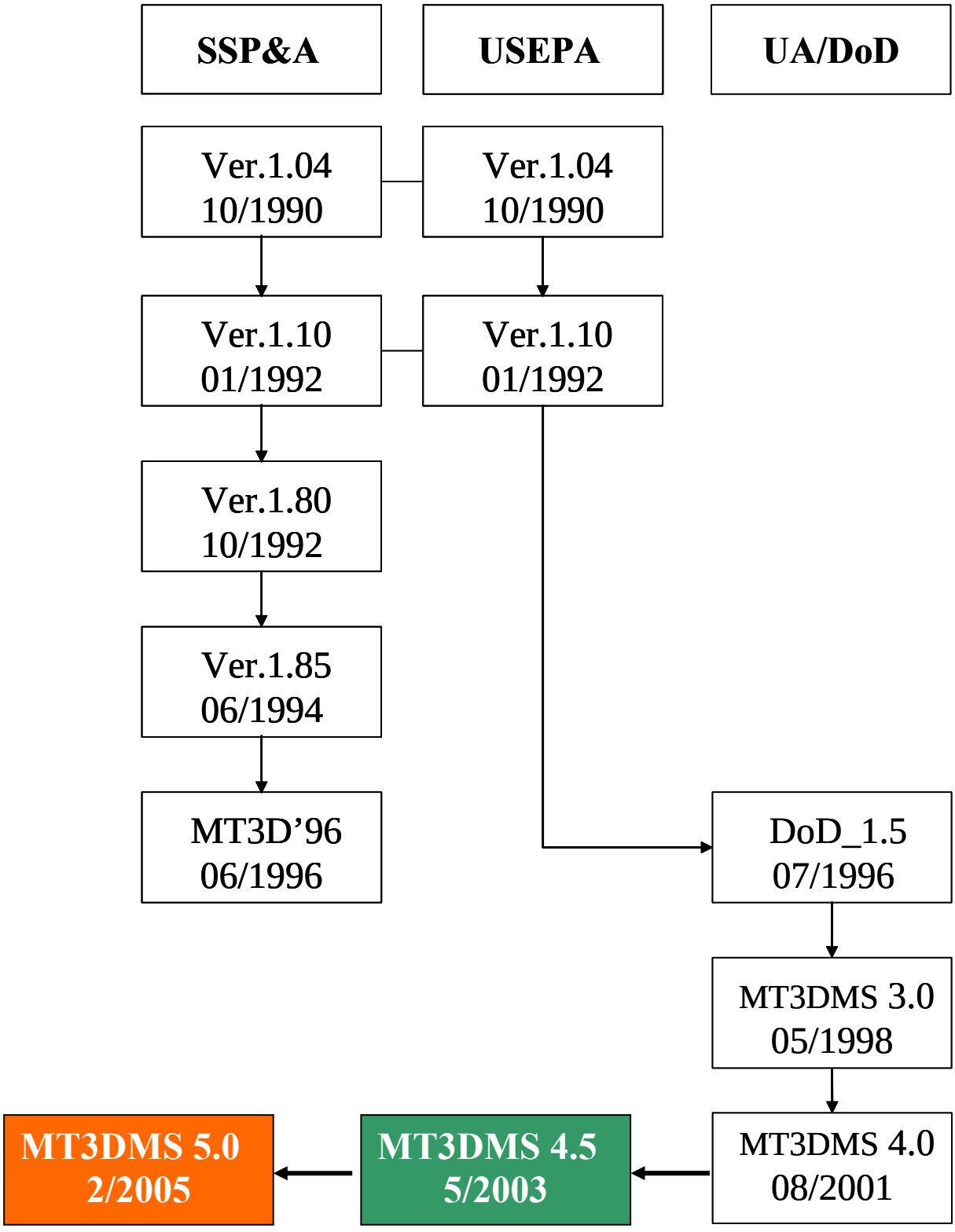
http://hydro.geo.ua.edu/mt3d/

and

http://www.mt3d.org

This lecture is based on slides created by Chunmiao Zheng and used when he lectured to this class in the past

A brief history of MT3D



Mathematical model of solute transport

- **Governing equations**
- **Initial conditions**
- **Boundary conditions**

SOLUTION TECHNIQUES:

Analytical: exact, closed form expression of head/concentration as function of space and time

Numerical: approximate estimation of head/concentration at discrete computational points through a numerical method

Governing equations

- **flow equation (as solved in MODFLOW)**

$$S_s \frac{\partial h}{\partial t} = \frac{\partial}{\partial x_i}\left(K_i \frac{\partial h}{\partial x_i} \right) + q_s$$

- **transport equation (as solved in MT3DMS)**

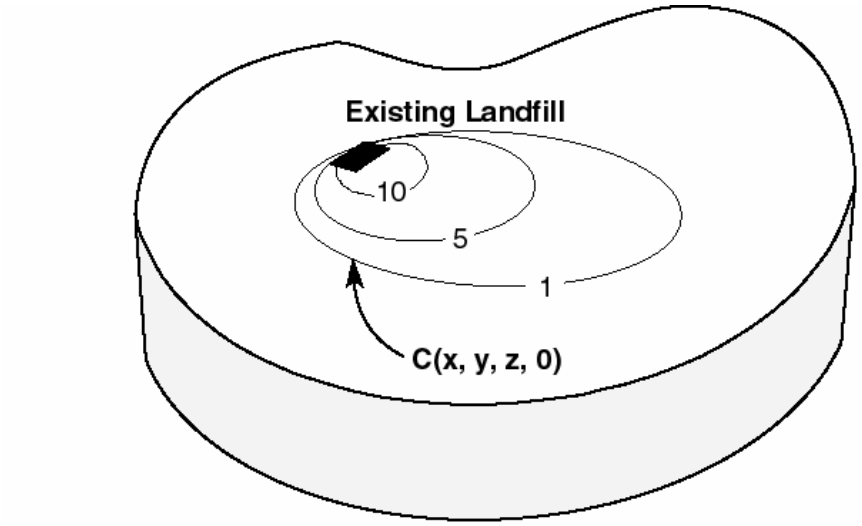
$$R\frac{\partial(\theta C)}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i}(q_i C) + q_s C_s + \boxed{\sum_{k=1}^{N} R_k}$$

$\leftarrow$ Chemical reaction term

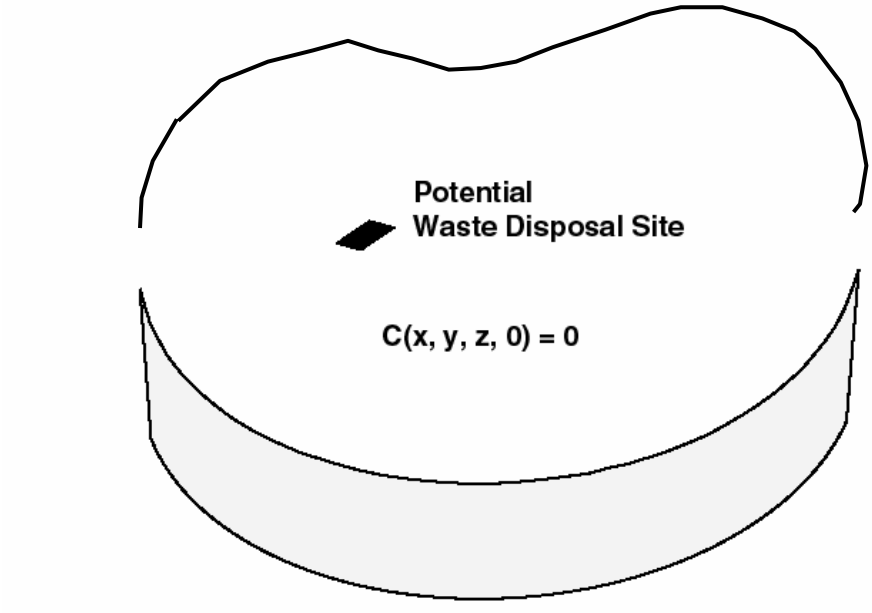
linkage between flow and transport

$$v_i = -\frac{K_i}{\theta}\frac{\partial h}{\partial x_i}$$

Initial conditions



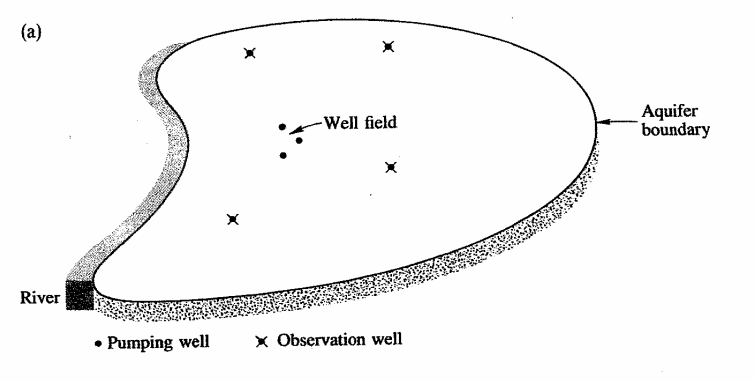
(a) Initial condition characterized by an existing plume.



(b) Initial condition characterized by zero concentration everywhere.

Boundary conditions

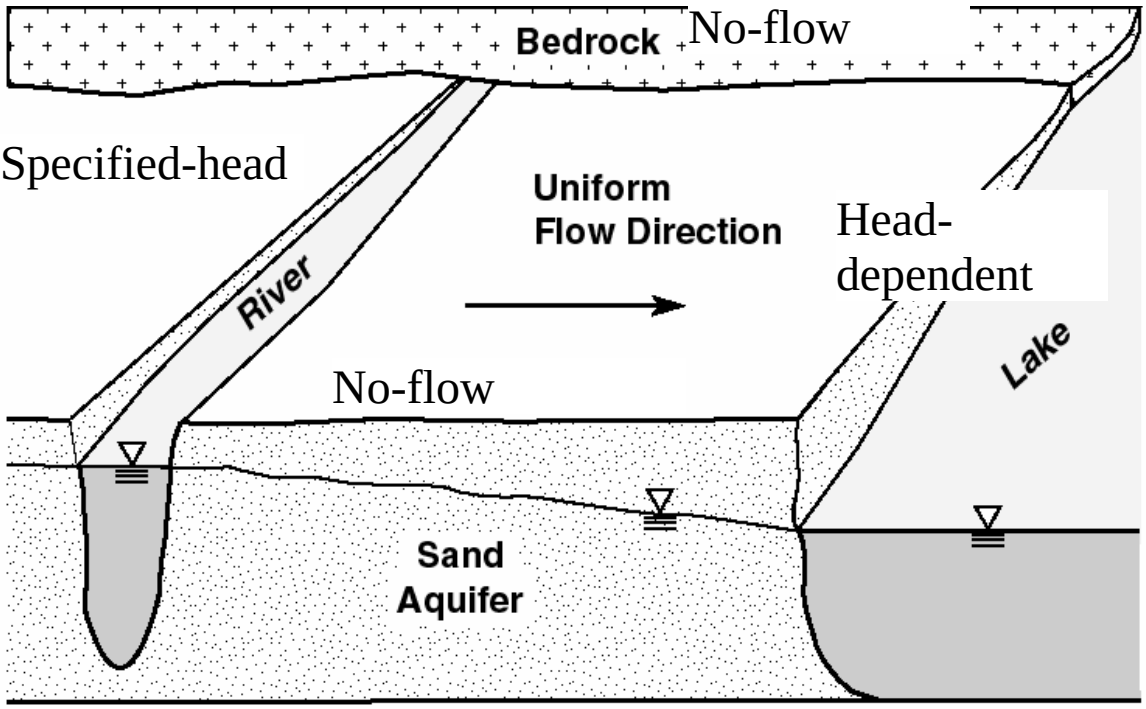
- **Constant-concentration [Dirichlet]**
- **Specified concentration gradient (i.e., dispersive flux) [Neumann]**
  ⇒*a special case is zero dispersive flux boundary*
- **Specified total mass flux (i.e., advective and dispersive)**
  ⇒*a special case is zero mass flux boundary*



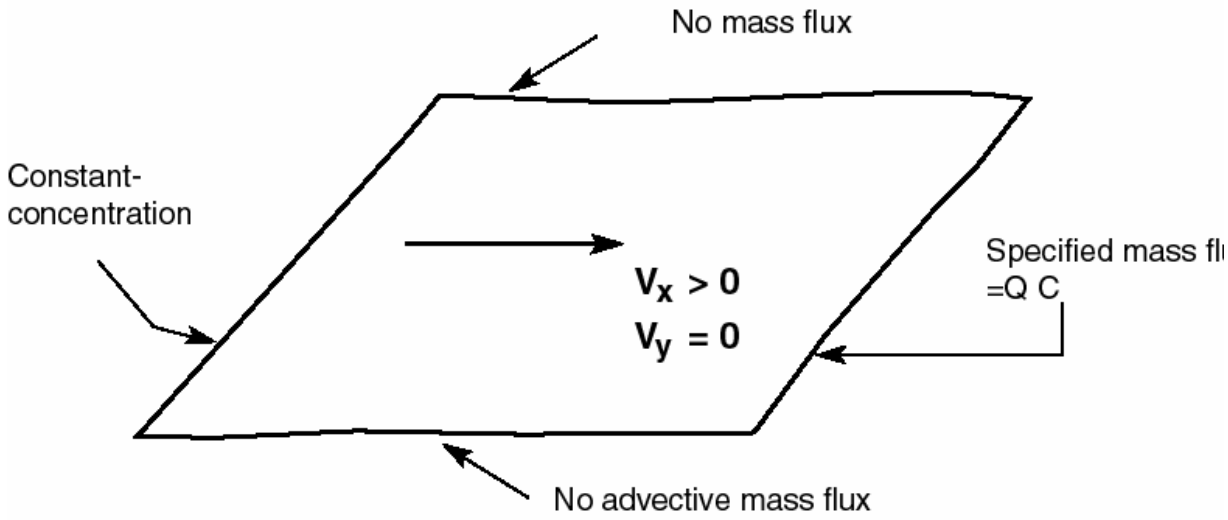
Notes:

⇒no-flow boundary in MODFLOW is automatically treated as zero mass flux boundary

⇒all other boundaries (including specified-flow; head-dependent; and constant-head) in MODFLOW are automatically treated as specified mass flux boundaries, with mass flux= QC, where Q may be specified by user or determined by MODFLOW. Dispersive flux across boundary is always assumed to be negligible.



(a) Hypothetical Flow System.



No dispersive flux in the simulation but may be in the field

(b) Transport Boundary Conditions.

Solution of the ADE

Advection-Dispersion Equation

$$R\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}\left(v_i C\right) + SSM + RCT$$

2^{nd} order 1^{st}-order

If porosity is not uniform

$$R\frac{\partial(\theta C)}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}\left(q_i C\right) + SSM + RCT$$

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

"Embarrassingly difficult…"
Mitchell (1984)

"…a problem no numerical method has fully overcome."
Baptista (1987)

Solution approaches

ADVECTION TERM

Multiple techniques

DISPERSION

SINK/SOURCE

CHEMICAL REACTION

Explicit Finite-Difference method (original MT3D)
Simple, but subject to time step-size constraint (no longer available in MT3DMS 5.0)

Implicit Finite-Difference method using the GCG Solver (MT3DMS)
Require a matrix solver, but no step-size constraint

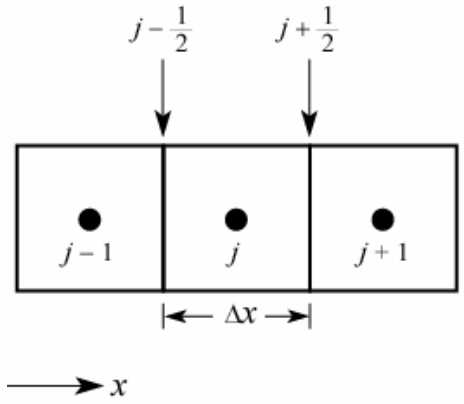
Solution techniques (advection term)

- **standard finite difference [FDM]**
  - **upstream weighting**
  - **central-in-space weighting**

- **method of characteristics [MOC]**
- **modified method of characteristics [MMOC]**
- **hybrid of method of characteristics [HMOC]**

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

Finite difference method



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

Difference in concentration gradients at the cell faces

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

Difference in concentration at the cell faces

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

$C_{j+1/2} = 0.5(C_j + C_{j+1})$ Central-in-Space

Substitution for weighting schemes in Implicit FDM

$C_{j+1/2} = C_{j-1}$ Upstream (Upwind)

Advantages and Disadvantages of FDM

- **advantages**

  $\Rightarrow$ mass conservative,

  $\Rightarrow$ computationally efficient for dispersion dominated problems,

  $\Rightarrow$ no numerical difficulty for distorted model grids or in the presence of many sinks/sources

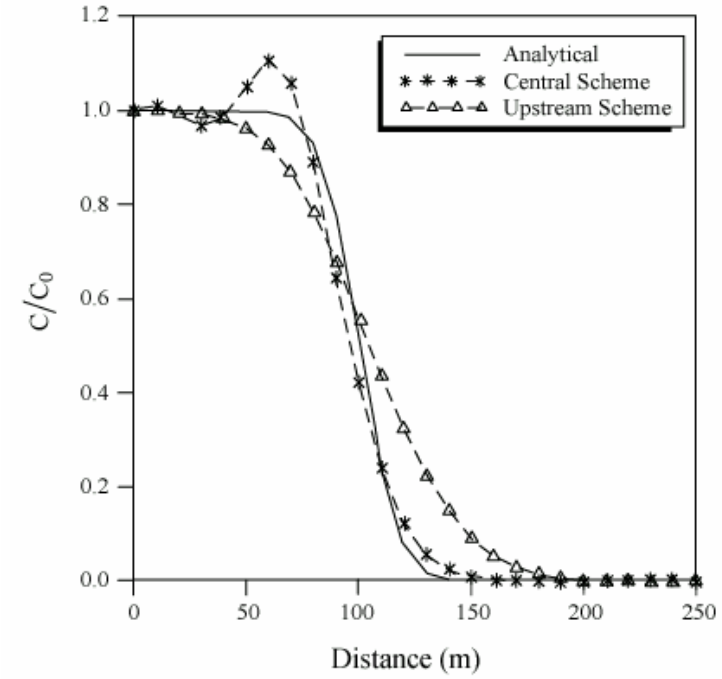
- **disadvantages**

  $\Rightarrow$ suffer from numerical dispersion errors for advection-dominated problems (upstream weighting) or from artificial oscillation (central-in-space weighting)

  $\Rightarrow$ to minimize numerical dispersion errors, fine spatial discretization may be necessary, i.e., to satisfy the Peclet number constraint:

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

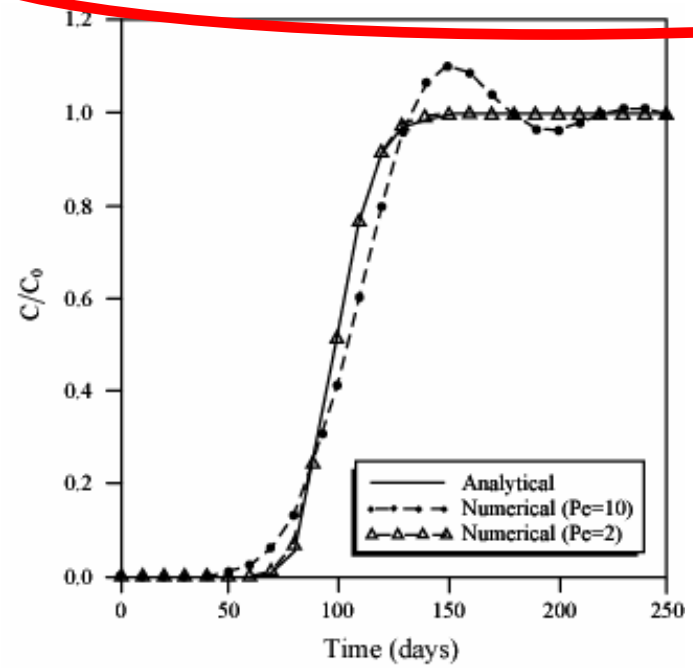
Illustration of numerical problems associated with central-in-space and upstream schemes



Central in Space FDM: Overshoot/Undershoot

Upwinding or Upstream Weighting FDM: Numerical dispersion

Effect of advection-domination (Peclet number)



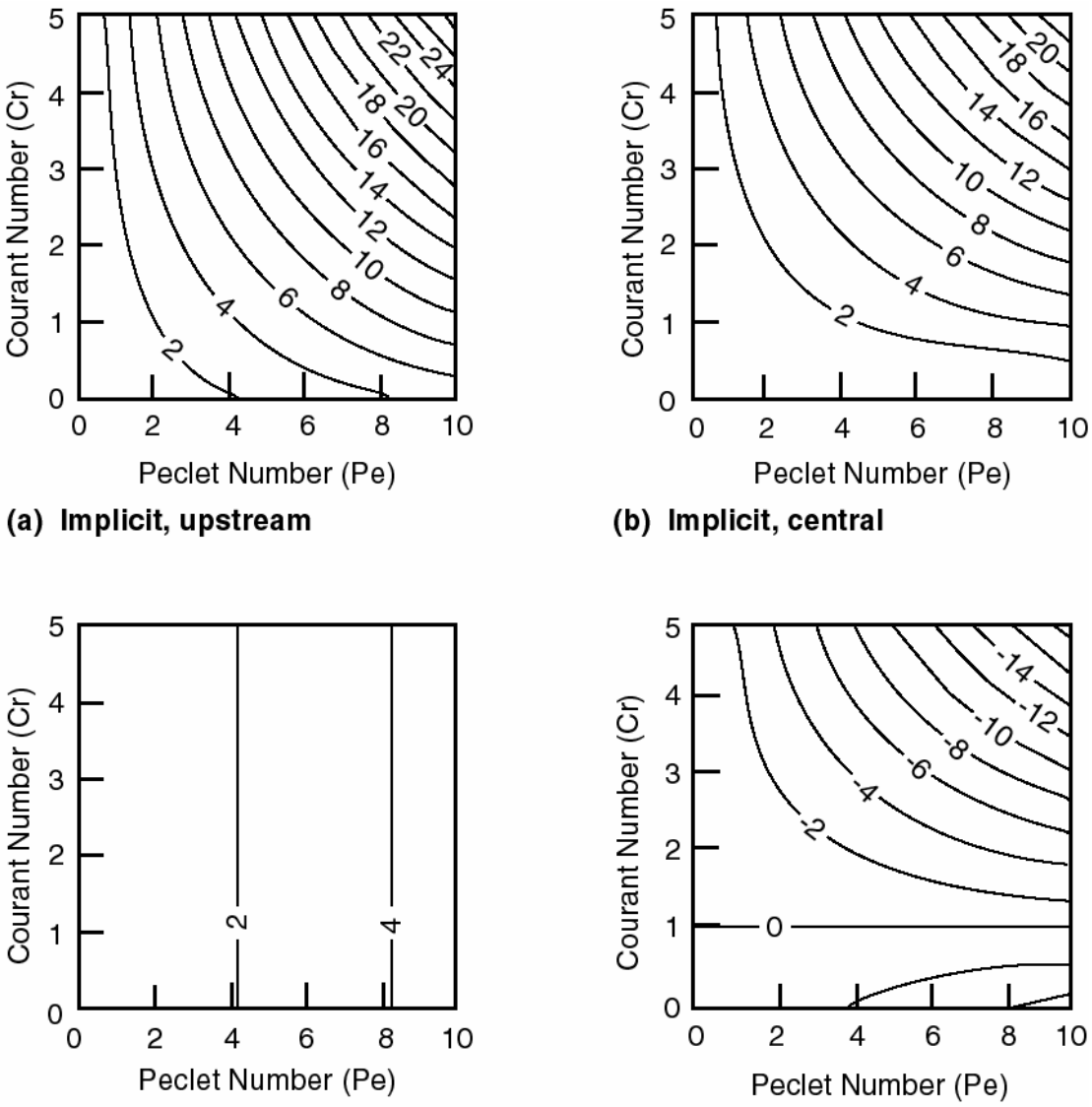


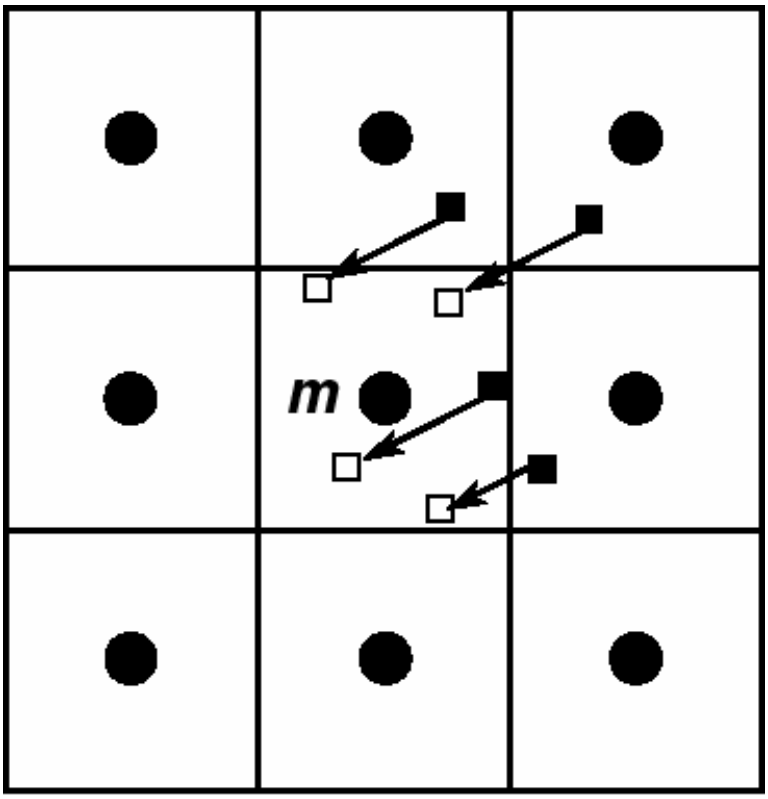
Figure 6-6. Ratio of numerical dispersion coefficient to physical dispersion coefficient as a function of the Peclet number and Courant number under four spatial and temporal discretization schemes

Courant number (*Cr*)

Number of cells an average particle will traverse in one time step

$$Cr = \frac{v_x \Delta t}{\Delta x} \qquad \Delta t = \frac{\Delta x Cr}{v_x}$$

Method of Characteristics (MOC)



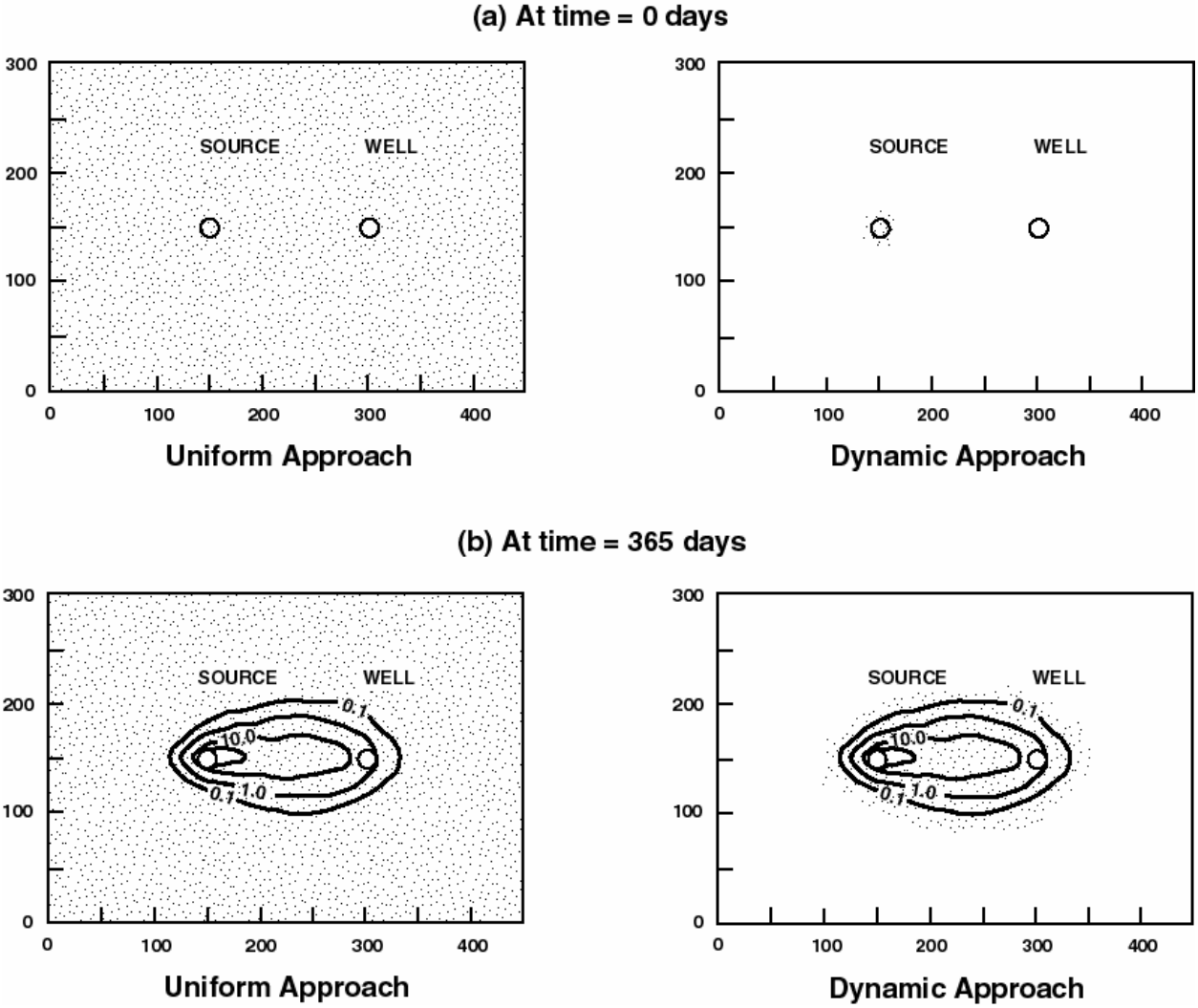
Each particle carries a volume and a concentration

Average C at next time step due only to advection

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

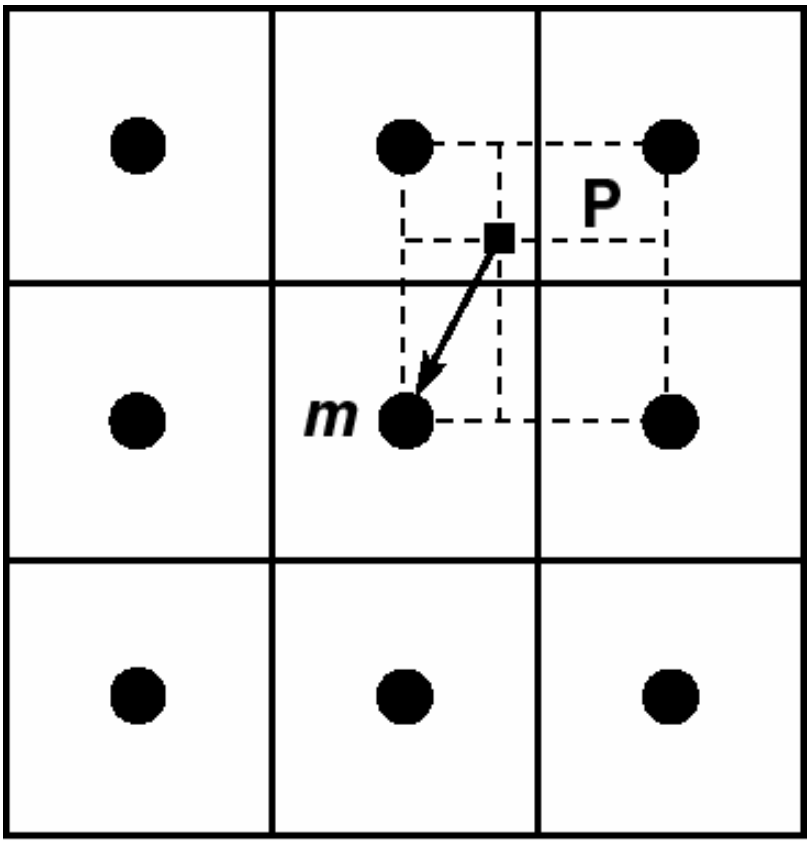
if volume υ_p is uniform

Particle allocation



Particle pattern: Random or fixed
NPL: number of particle per cell at low conc. gradient
NPH: number of particle per cell at high conc. gradient
DCEPS: critical concentration gradient for switching between NPL and NPH

Modified Method of Characteristics (MMOC)



Concentration at point *P* is interpolated from those at neighboring nodes

Calculate position backward from node to get advective C for next time step

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

Hybrid Method of Characteristics (HMOC)

vary the method in space as needed

- **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**

Advantages and Limitations of Particle Methods

- **advantages**

  $\Rightarrow$ virtually eliminate numerical dispersion

  $\Rightarrow$ computationally efficient for highly advection-dominated problems

- **disadvantages**

  $\Rightarrow$ may have mass balance discrepancy problems, particularly when the model grid is highly irregular

  $\Rightarrow$ calculated concentration breakthrough curves may be “rough”

  $\Rightarrow$ computer memory intensive, particularly for multi-species simulations, with a set of particles for each species

Third-order TVD (ULTIMATE)

Also referred to as higher-order finite-difference or finite-volume method

$$C_j^{n+1} = C_j^n - Cr\left(C_{j+1/2}^n - C_{j-1/2}^n\right)$$

where

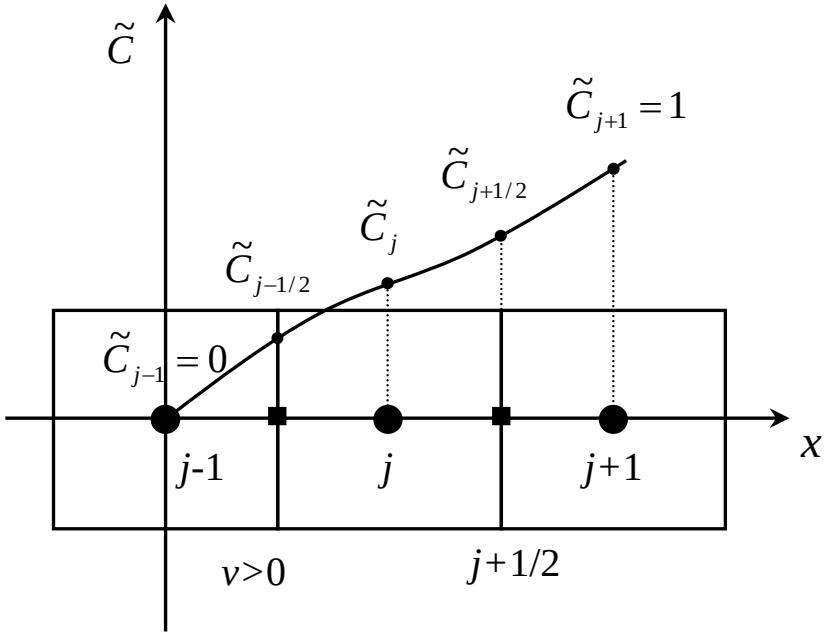
$$Cr = v\Delta t/\Delta x$$

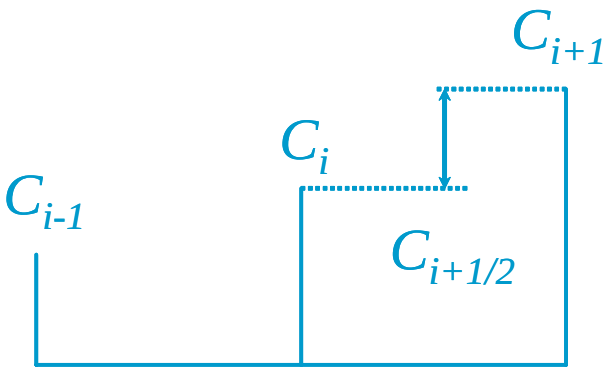
$$C_{j+1/2} = \left(C_{j+1} + C_j\right)/2 - Cr\left(C_{j+1} - C_j\right)/2 - \left(1 - Cr^2\right)\left(C_{j+1} - 2C_j + C_{j-1}\right)/6$$

$$C_{j-1/2} = \left(C_j + C_{j-1}\right)/2 - Cr\left(C_j - C_{j-1}\right)/2 - \left(1 - Cr^2\right)\left(C_j - 2C_{j-1} + C_{j-2}\right)/6$$

Improves FDM when grid is coarse or physical dispersion is small

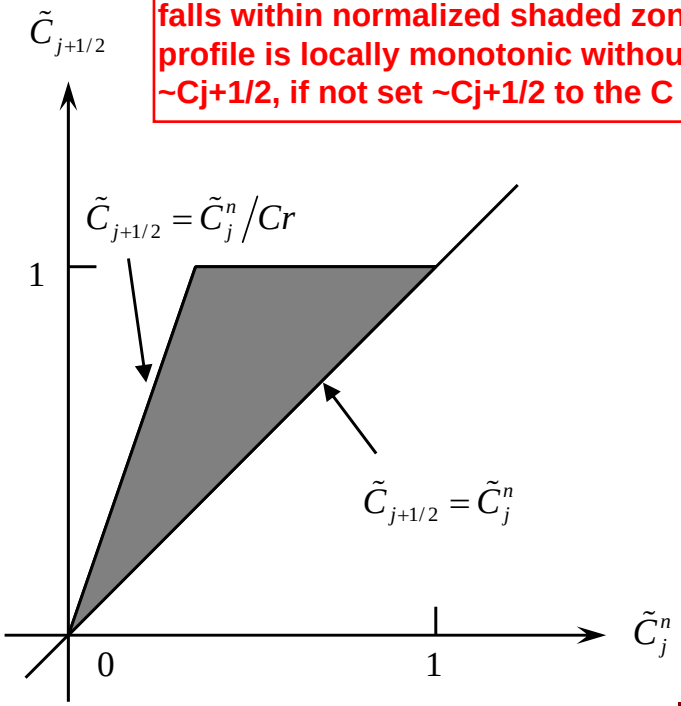
Model nodes used in 1D 3rd-order TVD





$$C_i \le C_{i+1/2} \le C_{i+1}$$

First check if concentration is monotonically increasing and determine if ~Cj+1/2 falls within normalized shaded zone shown below (i.e. check if concentration profile is locally monotonic without spurious oscillations). If so, proceed using ~Cj+1/2, if not set ~Cj+1/2 to the C value of closest upstream node



Flux limiter

Advantages and disadvantages of TVD

- **advantages**

  $\Rightarrow$ mass conservative

  $\Rightarrow$ minimal numerical dispersion and artificial oscillation for advection-dominated problems

  $\Rightarrow$ no numerical difficulty for distorted model grids or in the presence of many sinks/sources

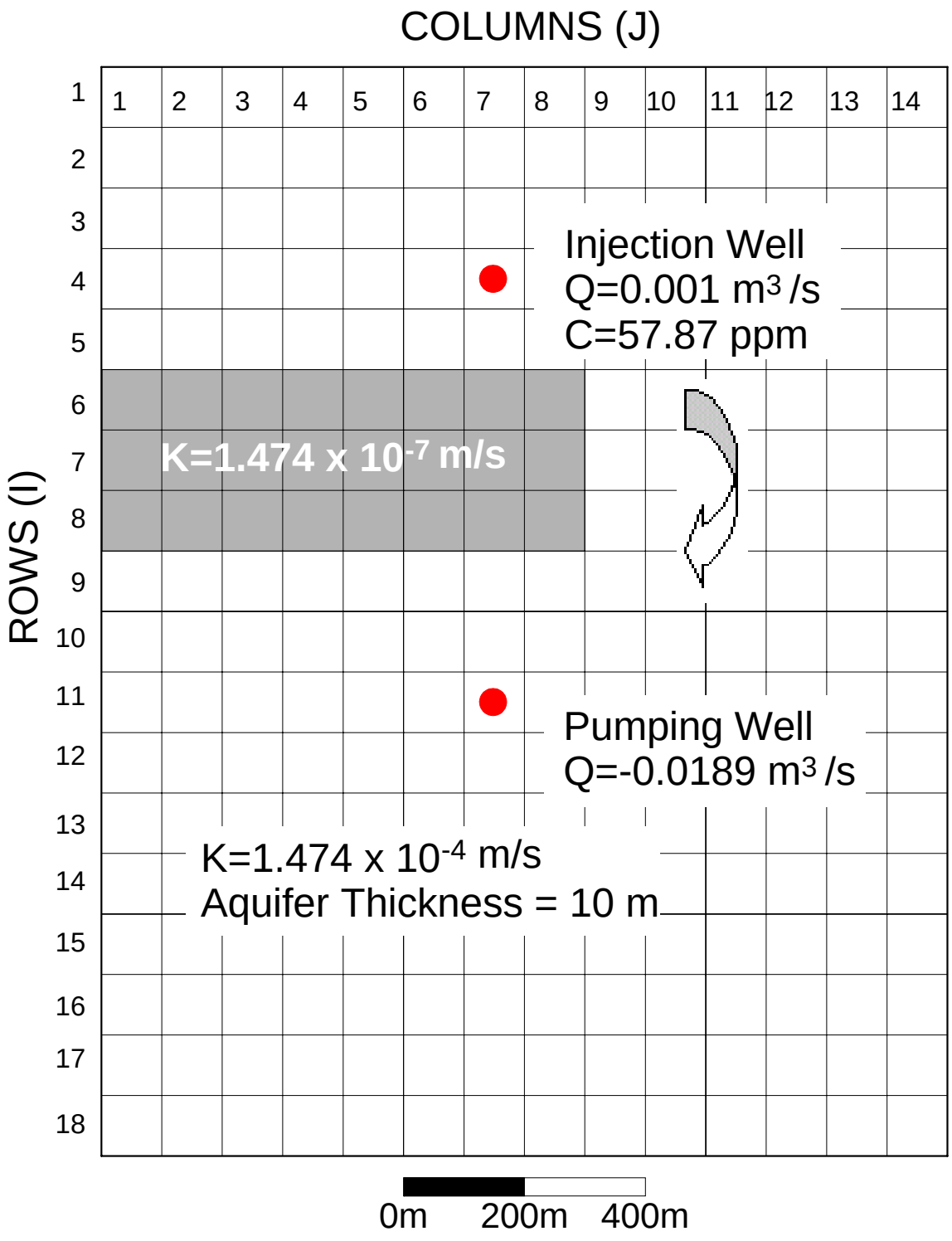
- **disadvantages**

  $\Rightarrow$ could be computationally demanding

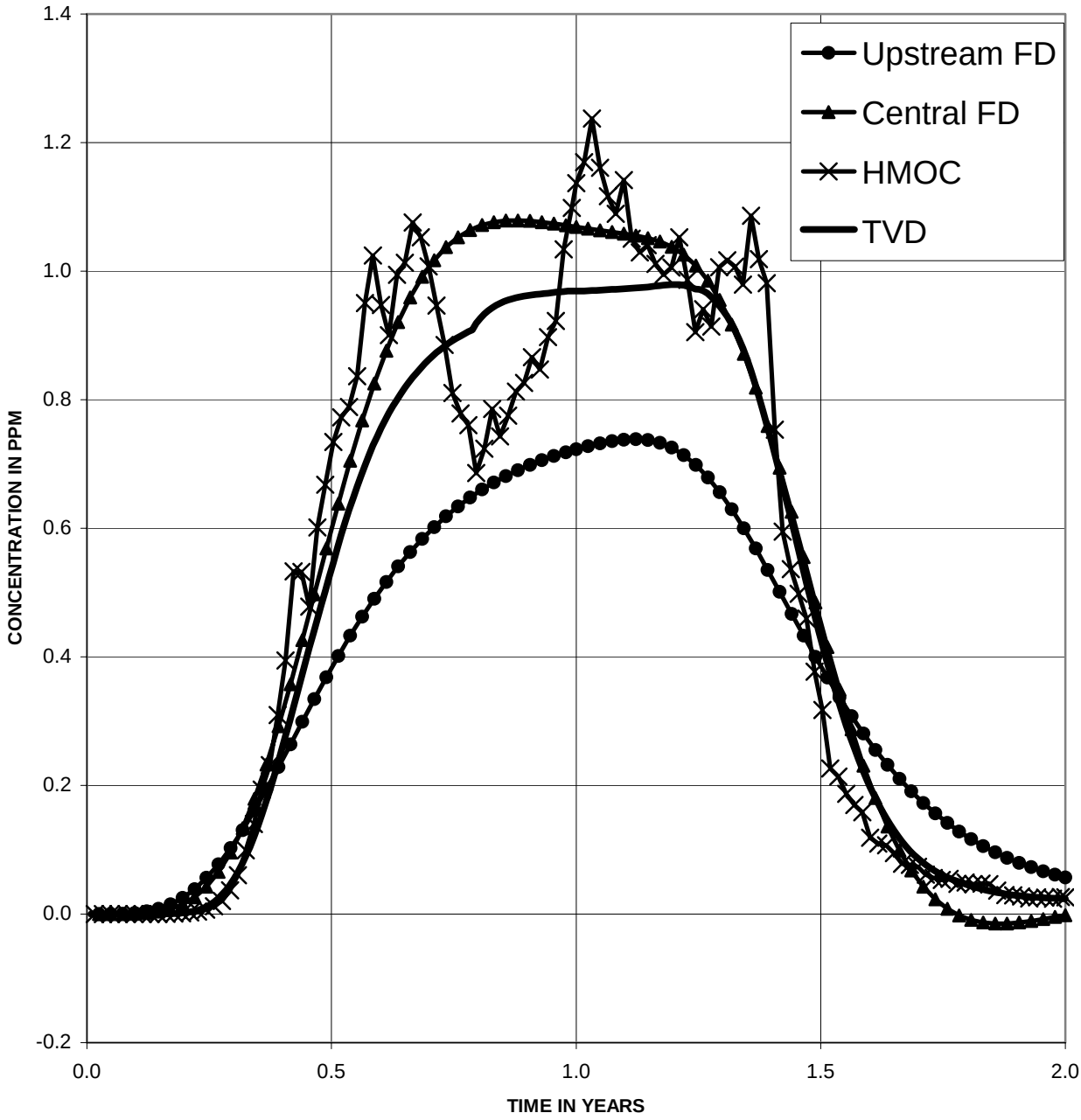
  $\Rightarrow$ may not be as effective as MOC in eliminating numerical dispersion for purely advective problems

Comparison of methods

-- a difficult problem

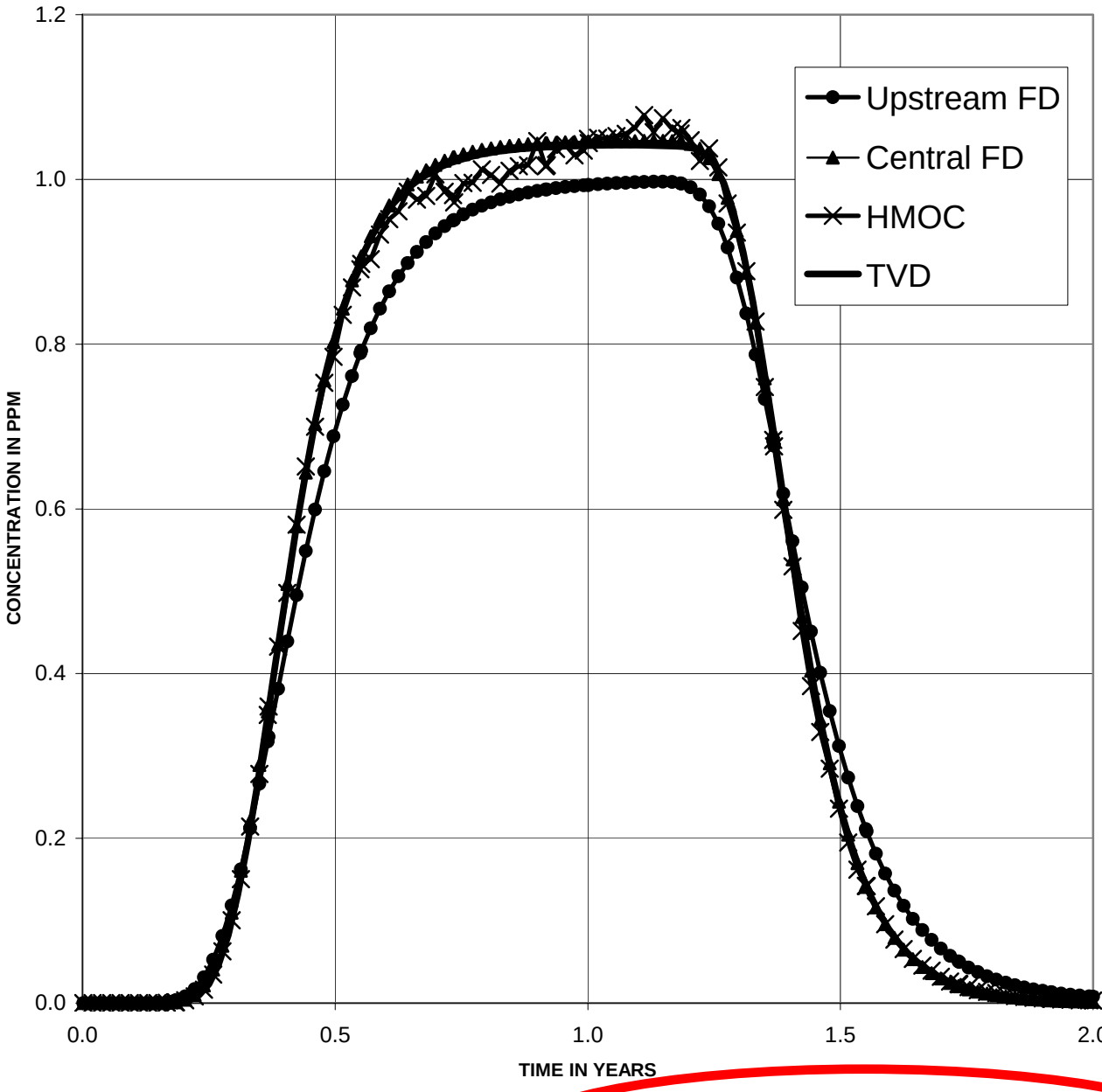


Comparison of calculated concentrations at the pumping well



$$Pe=\Delta x/\alpha_L=100/20=5$$

Comparison of calculated concentrations at the pumping well after grid refinement



$$Pe=\Delta x/\alpha_L=20/20=1$$

List of solution options in MT3DMS

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 Method
B	Particle Tracking Based Eulerian-Lagrangian Methods • MOC • MMOC • HMOC	*Implicit Finite-Difference Method*
C	Explicit Finite-Difference Method • Upstream weighting	Explicit Finite-Difference Method
D	*Implicit Finite-Difference Method* • *Upstream weighting* • *Central-in-space weighting*	*Implicit Finite-Difference Method*
E	*Explicit 3rd-order TVD (ULTIMATE)*	Explicit Finite-Difference Method
F	*Explicit 3rd-order TVD (ULTIMATE)*	*Implicit Finite-Difference Method*

Summary: classes of transport solution techniques

- **Eulerian**
  - **– Finite-difference**
  - **– Finite-element**
  - **– TVD**
- **Lagrangian**
  - **– Random walk**
- **Mixed Eulerian-Lagrangian**
  - **– MOC**
  - **– MMOC**
  - **– HMOC**

Fixed Grid

When Advection Dominates then
- **Overshoot**
- **Undershoot**
- **Numerical Dispersion**

Deforming Grid or Coordinates

Good for Pure Advection

Cumbersome for Dispersion

Use Eulerian for Advective Portion

Lagrangian for Dispersion

LESS EFFICIENT

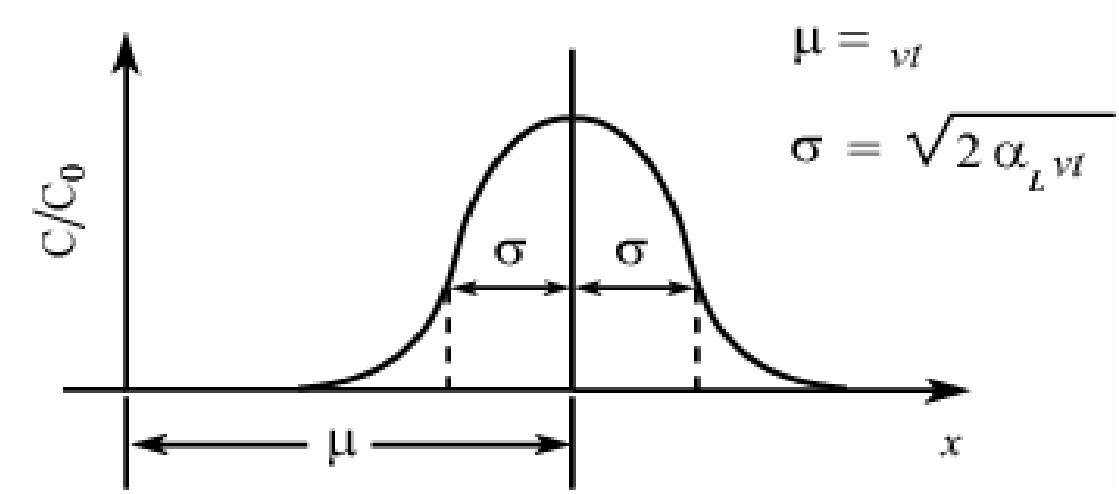
NOT MASS BALANCE BASED

"NTPack" from http://www.mt3d.org

5 programs using different transport techniques FDM FEM TVD MOC RW

Random walk method

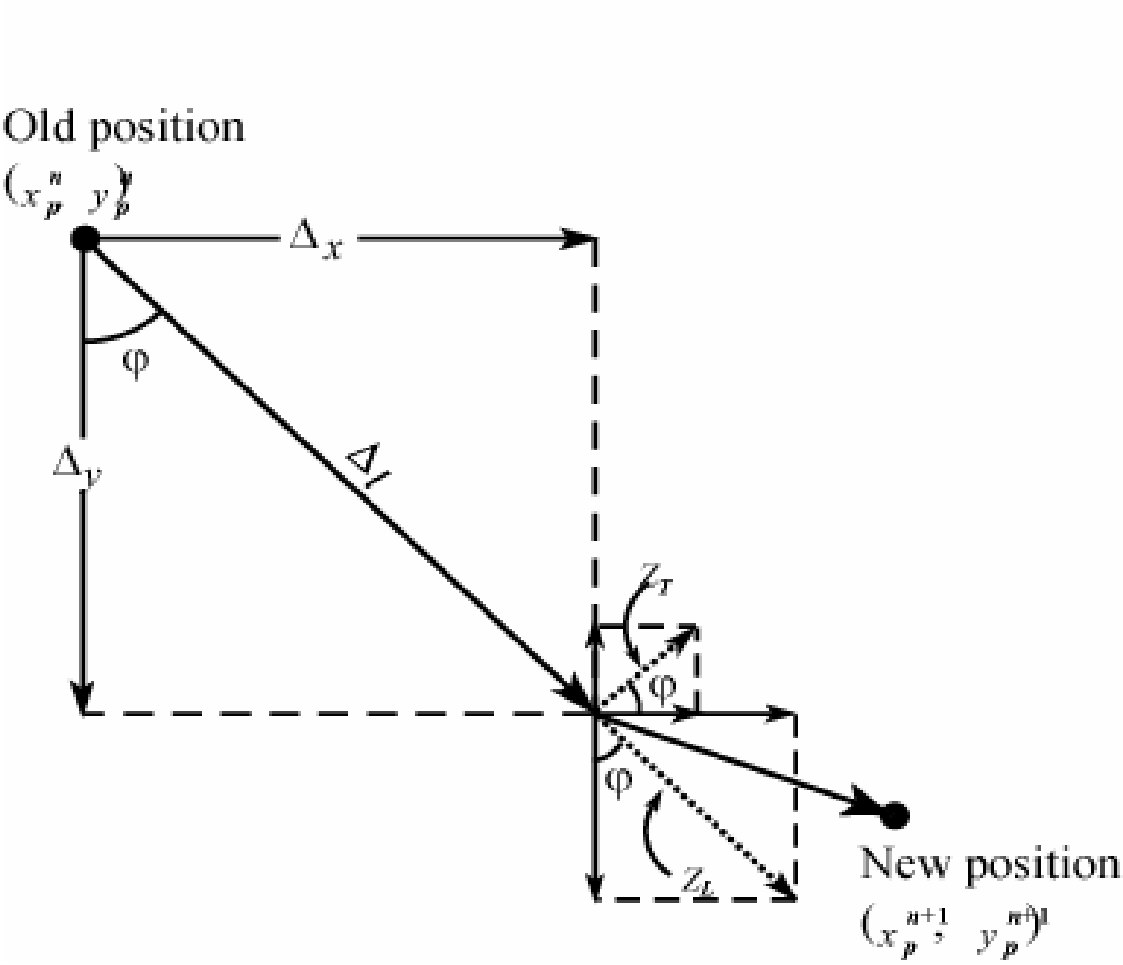
Basic concept



Normal probability density function (PDF)

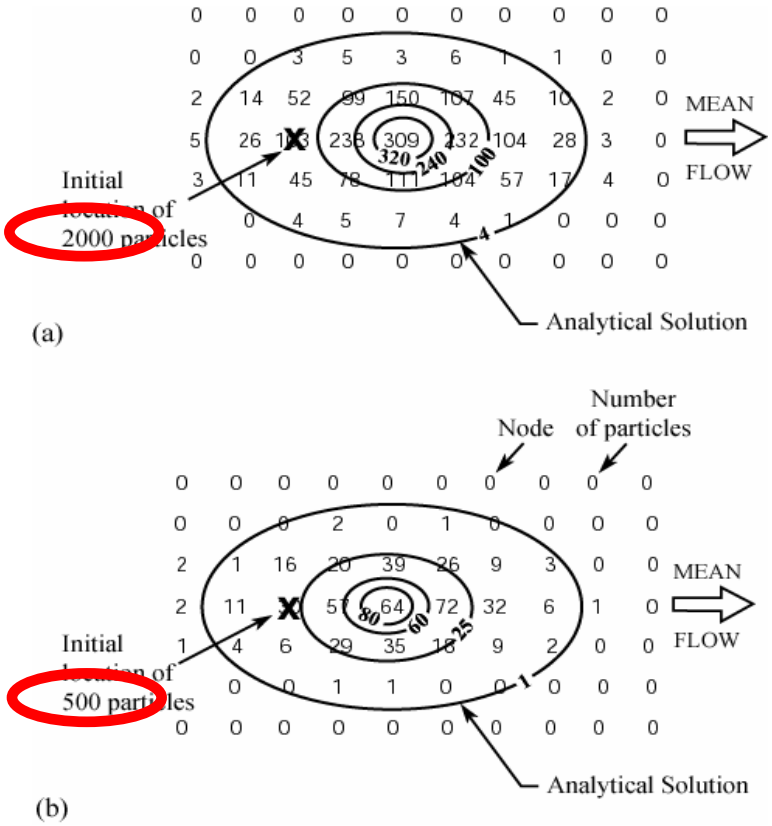
Random walk method

Illustration of a transport increment as a deterministic advective step and a random dispersive step



Random walk method

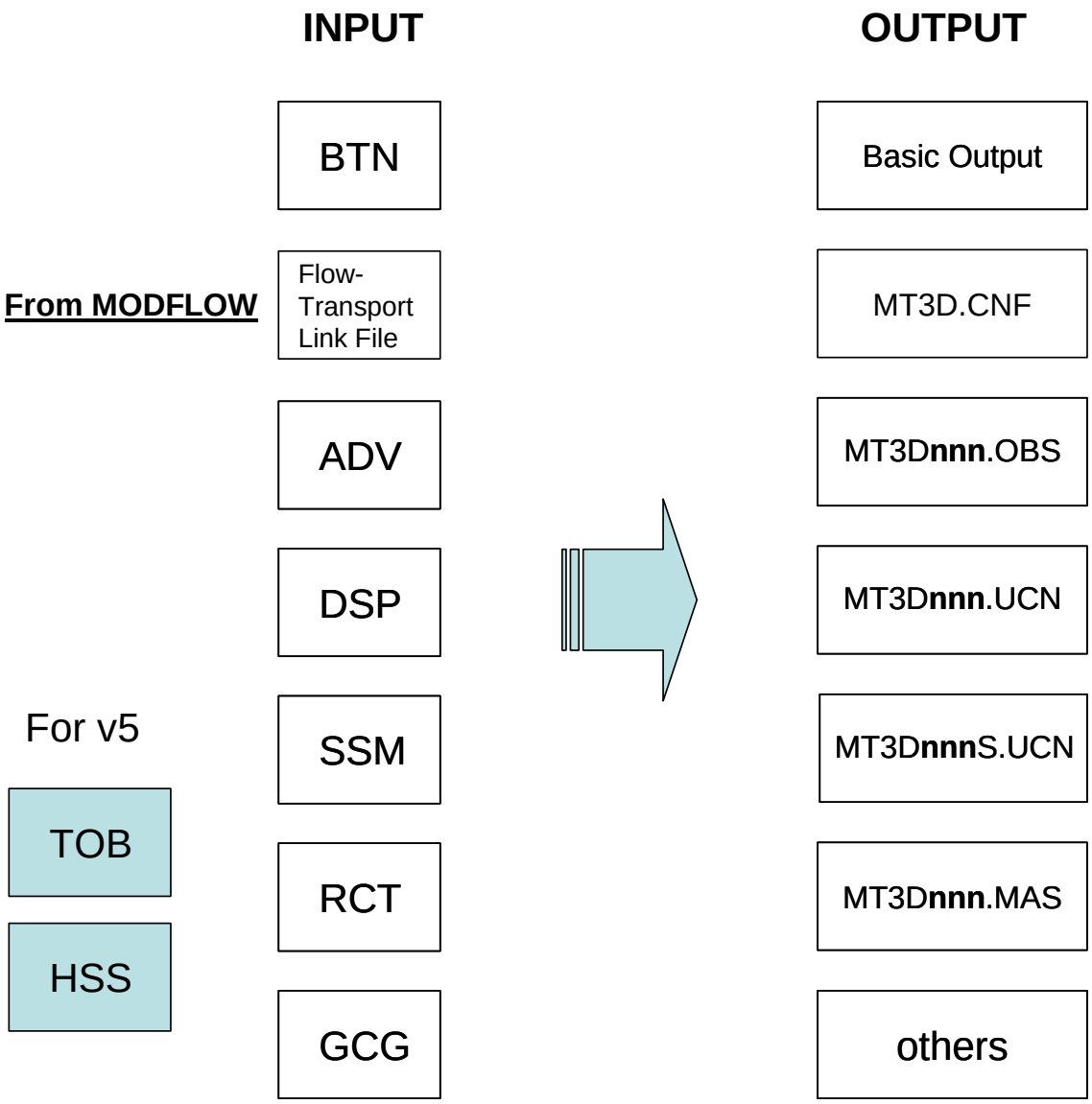
Concentration solution expressed in terms of particle distributions



Advantages: no numerical dispersion; efficient for advection-dominated problems

Disadvantages: sensitive to number of particles used; 'rough' solutions

MT3DMS file structure



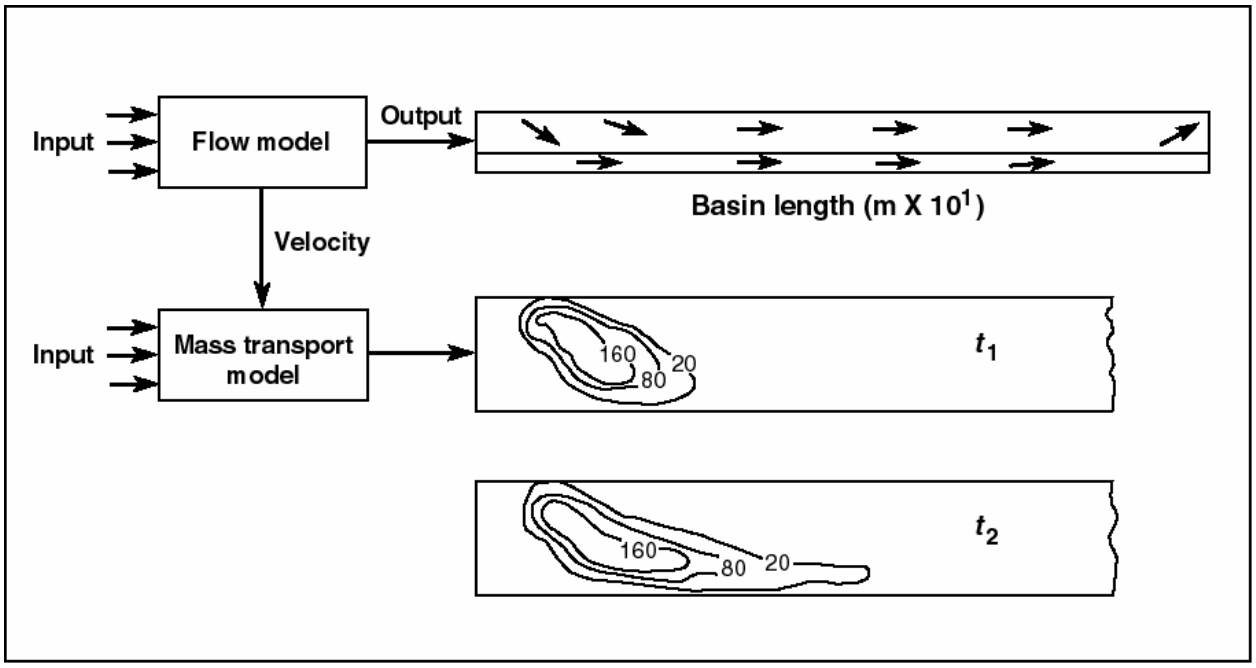
Use of units in mt3dms

1. The units for length and time used in MT3DMS simulation must be consistent, and match those used in MODFLOW. For example, if the following units are used in MODFLOW:
[Length]=m; [Time]=day

Then in MT3DMS the unit for dispersivity must be [m], and for first-order decay rate [day^{-1}]

2. The only exception to the above consistency rule is the unit for concentration, which may be arbitrary, as long as the user keeps the following points in mind:
(a) The output concentration unit is the same as the input unit;
(b) The mass calculated by MT3DMS based on inconsistent concentration unit must be converted if absolute mass value is important. The mass is calculated as product of $Q \times C \times \Delta t$; and
(c) No nonlinear reaction is simulated.
Otherwise, consistent units must be used for all variables, including concentration.

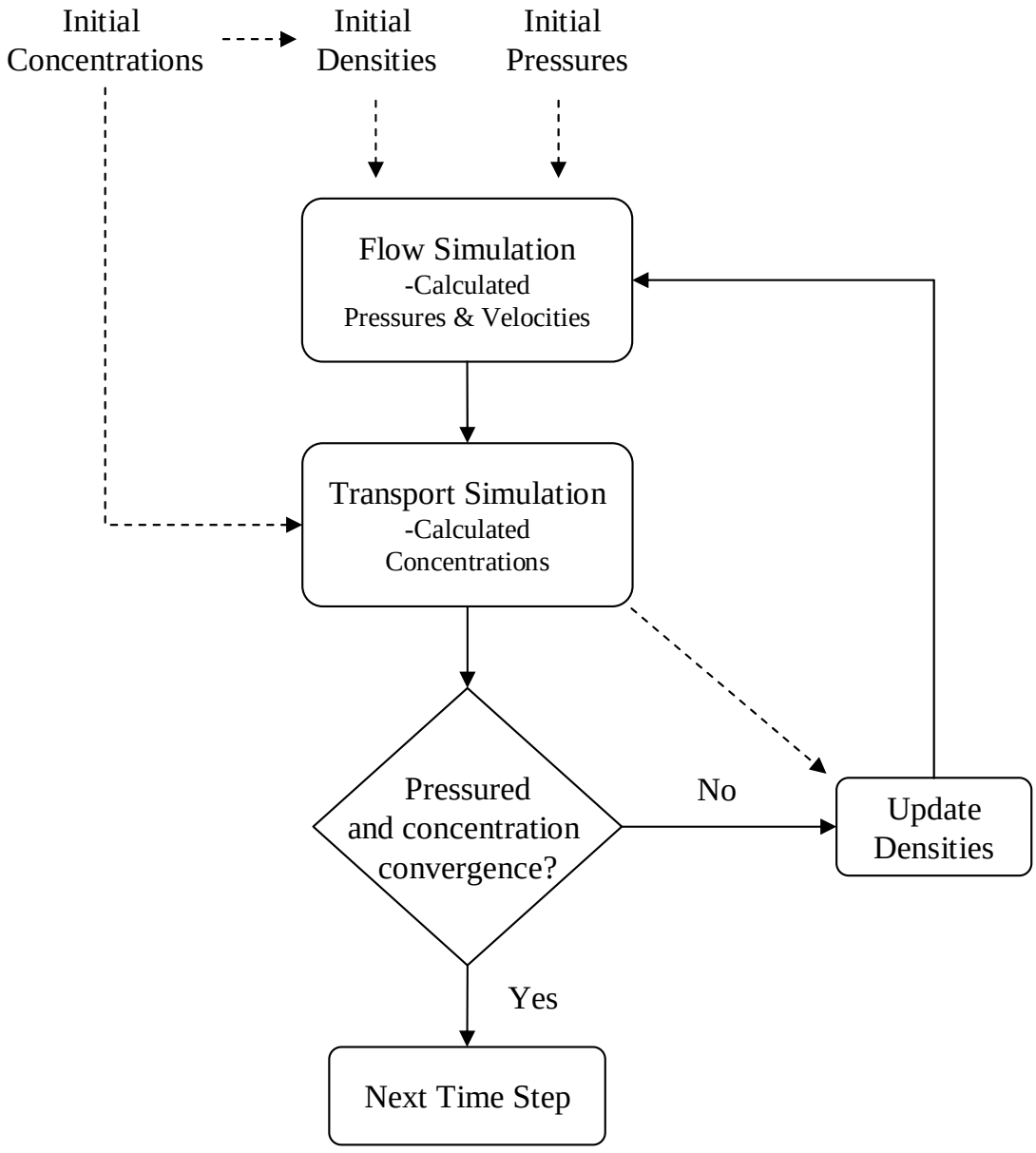
MODFLOW to MT3DMS linkage



Key assumption:
density change caused by solute transport is negligible

LMT package:
The LMT package is added to MODFLOW, which, when activated, saves velocity and sink/source information needed by MT3D

MODFLOW—MT3DMS linkage under variable water density



Steps in running mt3dms

- **Run MODFLOW**
  ⇒Save MODFLOW-MT3DMS link file by activating the LMT package added to MODFLOW

- **Create MT3DMS input files (text editor or a preprocessor)**

- **Run MT3DMS**
  ⇒Set appropriate output control options in MT3DMS to save the unformatted concentration file and/or the observation file

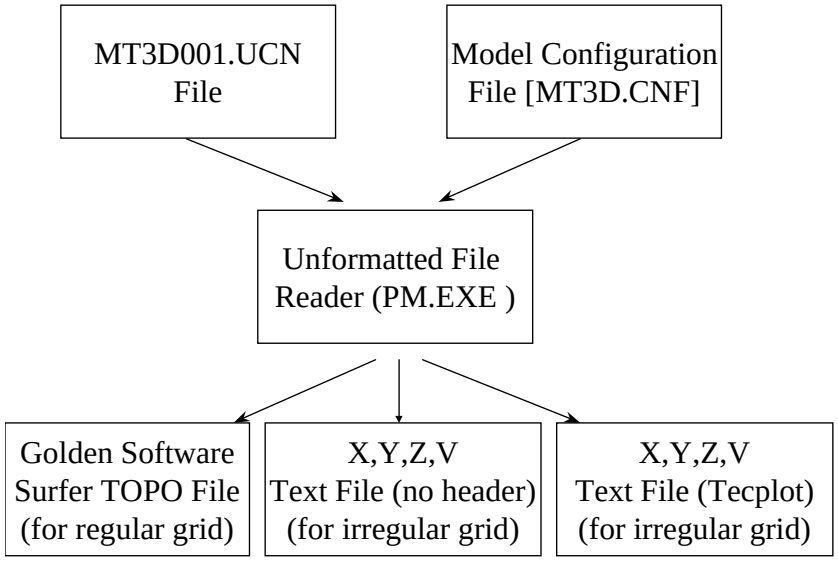
- **Post-process (using a post-processor or an external graphic package in conjunction with a file translation utility)**

Postprocessing mt3dms

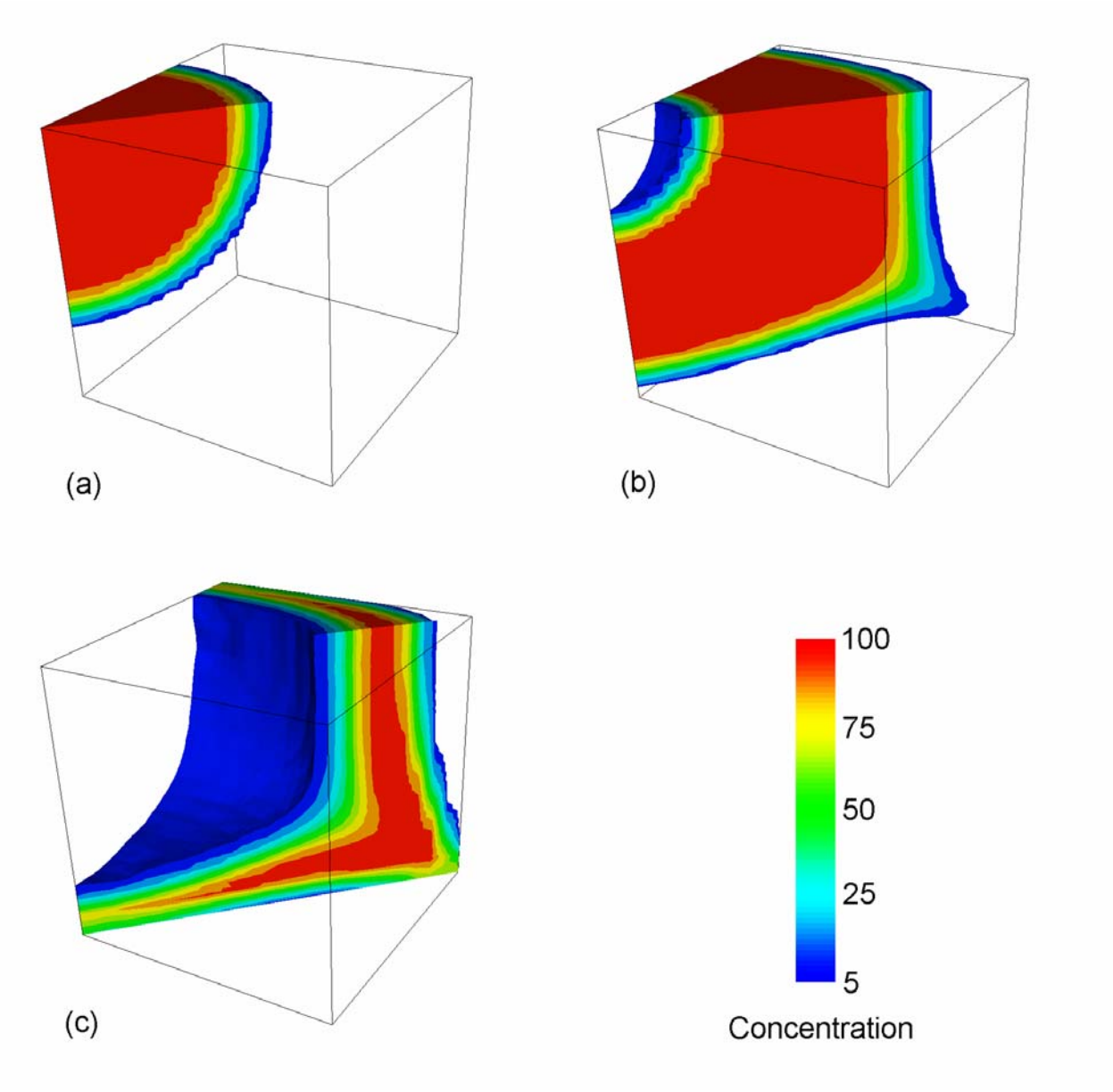
- **Breakthrough curves at specified observation points:**

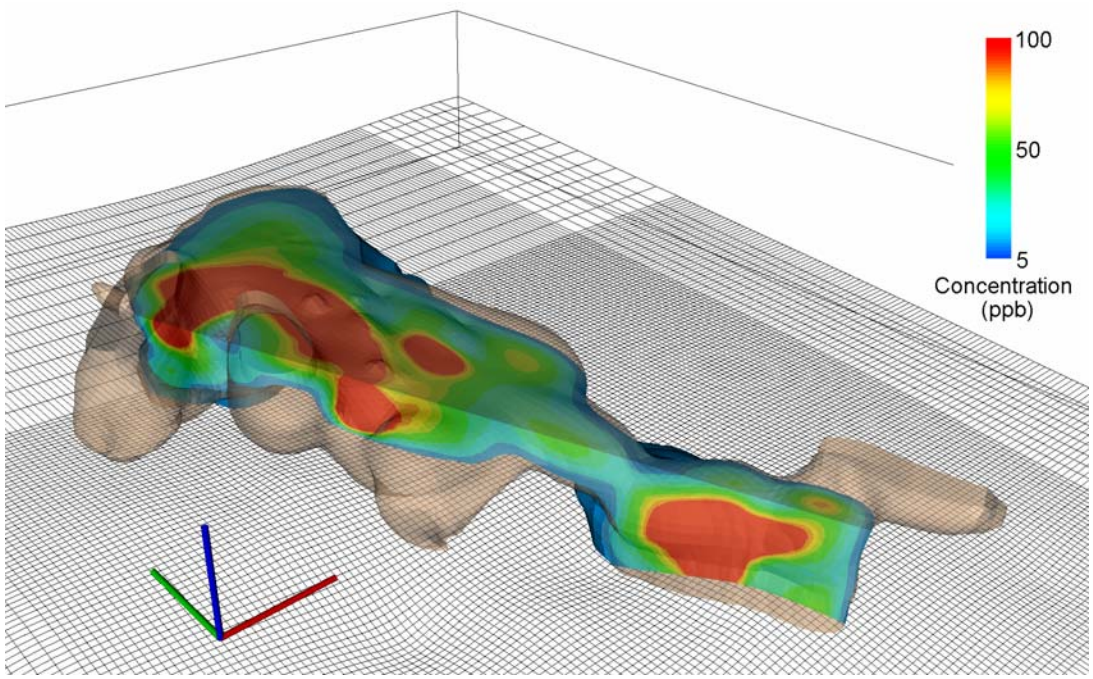
  MT3DXXX.OBS →spreadsheet, x-y graphing packages

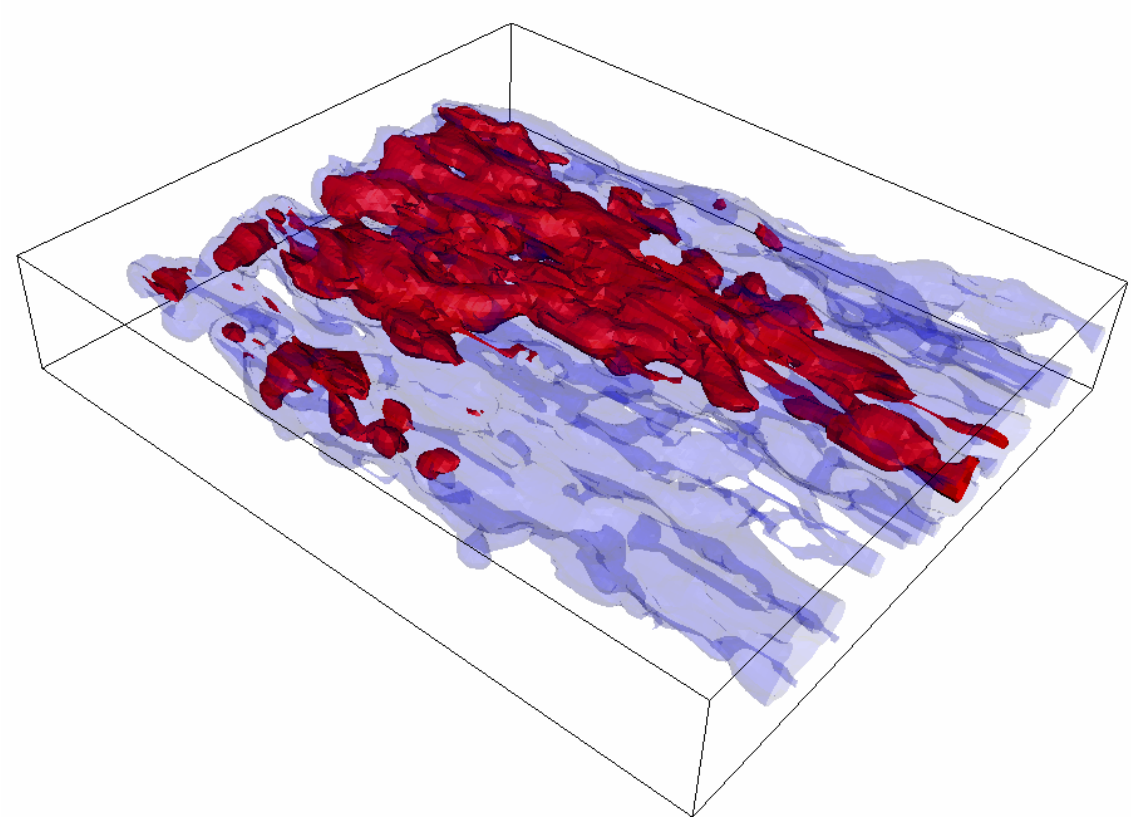
- **Plan view or cross sectional concentration contour maps:**



USGS Model Viewer




100
50
5
Concentration
(ppb)



Basic Transport Package

Purpose

To specify:

- Basic information
- Spatial discretization
- Boundary and initial conditions
- Printing and saving options (output control)
- Temporal discretization

Basic Transport Package

- Model Layer Type (LAYCON):

  =0: confined layer

  ≠0: unconfined or convertible

Case	ModFlow	MT3D
Confined	0	0
Unconfined	1	1
Convertible	3	1
Convertible w/ constant T	2	1

IMPLICATIONS

- LAYCON=0: user-specified DZ used as saturated thickness
- LAYCON ≠0: MT3D determines saturated thickness internally as MODFLOW

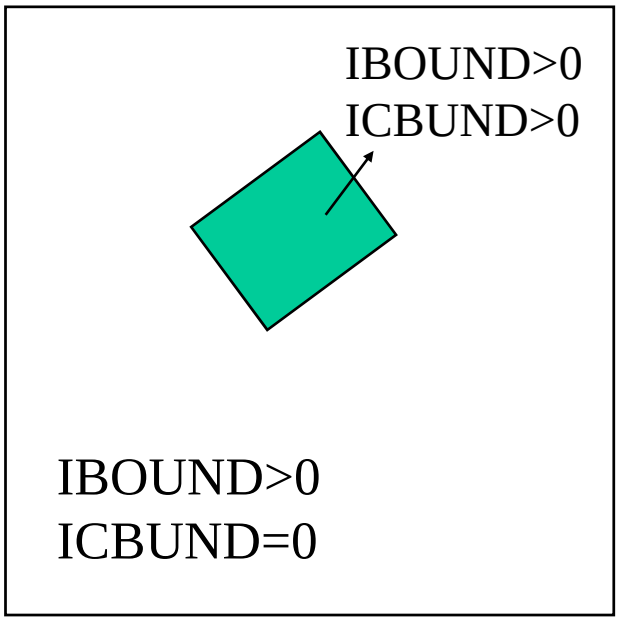
Basic Transport Package

- HTOP: top elevation of the 1st model layer
  - If top layer is confined, the HTOP values correspond to the actual top elevations of layer 1
  - If top layer is unconfined, HTOP can be set to arbitrary values, but keep in mind:
    - (HTOP - DZ1) ≡ BOT1 (bottom elevation of layer 1 as specified in MODFLOW)
    - Concentration for top layer is calculated midway between HTOP and BOT1

Basic Transport Package

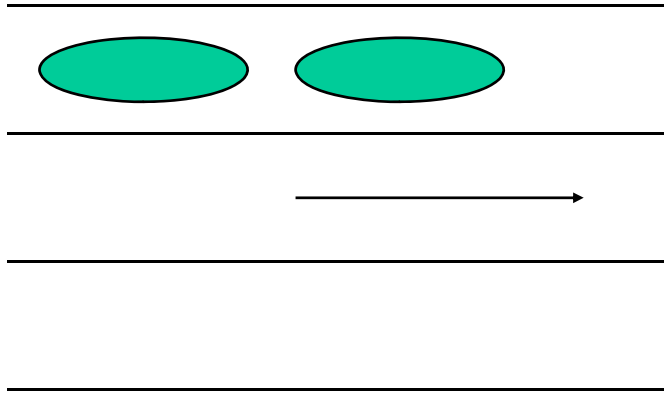
- IBOUND vs. ICBUND

  Active cells in MODFLOW (IBOUND>0) may be defined as inactive cells in MT3D (ICBUND=0) to speed up transport computation



Basic Transport Package

- Vertical resolution



Basic Transport Package

- Temporal discretization
  - If flow model is steady-state and has ONLY one stress period, transport model can have as many stress periods as necessary, with any desired length for each stress period
  - For all other situations, the number of stress periods (NPER), the number of [flow] time steps in each stress period (NSTP) and the time step multiplier (TSMULT) must be identical in flow and transport models

Basic Transport Package

- For each stress period
  - PERLEN (same as in MODFLOW)
  - NSTP (same as in MODFLOW)
  - TSMULT (same as in MODFLOW)
  - TSLNGH(NSTP) (only for a flow model other than MODFLOW)
  - DT0: maximum allowable transport stepsize

  [NEW IN MT3DMS]
  - TTSMULT: transport stepsize multiplier within a flow-model time step
  - TTSMAX: maximum transport stepsize within a flow-model time step

Advection Package

Purpose

- Solve the advection components of the transport equation, using one of the following options (through input variable `MIXELM`):
  - Finite Difference (FDM)
  - MOC (method of characteristics)
  - MMOC (modified MOC)
  - HMOC (hybrid MOC/MMOC)
  - TVD (ULTIMATE)

Advection Package

Allowable step size for advection

- the Courant number, C_r (input variable PERCEL) controls the number of cells any particle is allowed to move during one transport step:

$$\Delta t_{ADV} = C_r \min\left(\frac{\Delta x}{|v_x|}, \frac{\Delta y}{|v_y|}, \frac{\Delta z}{|v_z|}\right)$$

  Δt_{ADV} is automatically multiplied by retardation factor, R, if sorption is simulated.

- MOC, MMOC, HMOC: $C_r \geq 1$, (generally set equal to 1.0)
- Explicit 3rd order TVD: $C_r \leq 1$ (generally set equal to 0.5~1.0)

Advection Package

- In MT3DMS, a fully implicit finite-difference option (for ALL terms including advection, dispersion, sink/source, reaction) is available to solve the advection term **WITHOUT** any stepsize limitation. However, for accuracy reasons, the Courant number should not be much greater than one, if the problem is advection-dominated.

Advection Package

1) MOC

- ITRACK = 1 generally OK (1st order)
  = 2 generally overkill (RK4)
  = 3 suggested (combination)
- WD $0.5 \leq WD \leq 1.0$
  = 0.5 generally OK
  = 1.0 purely advective transport
- DCEPS $= 10^{-5}$ generally OK
- NPLANE = 0 (random pattern), generally adequate
  ≠ 0 for relatively uniform flow
  = 1: 2D plan
  = 2-3: cross section or 3D
- NPL = 0 generally OK, may be as many as NPH
- NPH ≤ 16 generally OK for 2D
  ≤ 32 generally OK for 3D
- NPMIN 0 to 4 generally OK
- NPMAX $\approx 2 \times NPH$
- SRMULT = 1

2) MMOC

- INTERP = 1 only option available
- NLSINK = NPLANE generally OK
- NPSINK = NPH generally OK

3) HMOC

- DCHMOC $= 10^{-3}$ generally OK

Dispersion Package

Purpose

- Solve the dispersion component of the transport equation, using the finite-difference technique
- Explicit scheme is subject to a maximum transport stepsize of

$$\Delta t_{DSP} \leq \frac{0.5\ R}{D_{xx}/(\Delta x)^2 + D_{yy}/(\Delta y)^2 + D_{zz}/(\Delta z)^2}$$

- Implicit scheme (GCG solver) has NO stepsize limit

Dispersion Package

DSP Package Input

- AL (longitudinal dispersivity, unit L)
  - cell-by-cell
  - 2D array for each model layer
- TRPT (ratio of horizontal transverse dispersivity vs longitudinal dispersivity)
  - one value per model layer
  - input as 1D array for all layers
- TRPV (ratio of vertical transverse dispersivity vs longitudinal dispersivity)
  - one value per model layer
  - input as 1D array for all layers
- DMCOEF (effective diffusion coeff., D^*)
  - one value per model layer
  - input as 1D array for all layers
  - $D^*=\tau D_o$ where τ I is tortuosity and D_o free-solution diffusion coefficient)

Dispersion Package

- Literature review (see Zheng/Bennett, Chapter 9)
- Things to consider
  - more heterogeneity included in flow model, smaller dispersivities are needed in transport model
  - scale dependent, but at what scale is problem specific
  - rules of thumb:
    TRPT: 0.1-0.01
    TRPV: 0.01-0.001
  - temporal variations can account for significant amount of dispersion
  - *is dual-domain mass transfer model more appropriate?*

Sink/Source Mixing Package

Purpose

- Solve the source and sink components of the transport equation, using the explicit finite difference method, subject to a stability constraint of

$$\Delta t \leq \min\left(R\theta / q_s\right)$$

  NOTE: q_s is the volumetric sink/source flow rate divided by the cell volume
- In MT3DMS, the implicit scheme can be used to solve the sink/source components WITHOUT the stability constraint

Sink/Source Mixing Package

- Specify hydraulic sinks and sources

  I. POINT SINKS/SOURCES

  – **constant-head cells** [ITYPE=1]
  – wells [ITYPE=2]
  – drains [ITYPE= 3]
  – rivers (or streams) [ITYPE=4]
  – general-head-boundary cells [ITYPE=5]
  – ……

  II. DISTRIBUTED SINKS/SOURCES

  – recharge
  – evapotranspiration

Sink/Source Mixing Package

- What's MXSS?
  - The maximum number of POINT sink/source cells (including constant-head cells) used in the flow model. It is used only for memory allocation memory purposes.
- How does MT3D know about the cell locations and flow rates of sinks/sources?
  - Through the flow-transport link file saved by the Link-MT3D package added to MODFLOW

Sink/Source Mixing Package

- Time-varying constant-concentration cell [ITYPE= –1]
  - this overrides the constant-concentration condition as defined in the BTN input [ICBUND<0]
  - once a cell is defined as ITYPE= –1, it remains a constant-concentration cell, but a new concentration value can be specified in different stress periods
- Mass-loading source cell [ITYPE=15]
  - Users specify Q*C directly [MT^{-1}]

Sink/Source Mixing Package

- Specify concentrations of sinks and sources

  I. SINKS

  – by default, concentration of all sinks set equal to that of aquifer at sink cell locations

  – default concentration of all sinks cannot be changed except for evapotranspiration

  II. SOURCES

  – by default, concentration of all sources set equal to ZERO unless specified by the user

Sink/Source Mixing Package

- Constant-head vs. Constant-Concentration
  - A constant-head cell in MODFLOW is treated as a regular fluid sink/source (like a well), the net inflow/outflow rate through the constant-head cell is determined internally by MODFLOW.
  - If the constant-head cell acts as a source (inflow), the source concentration is zero unless specified by the user in SSM input. If it acts as a sink (outflow), the sink concentration is always equal to that of aquifer.
  - A constant-head cell can be specified as a constant-concentration if so desired.

Chemical Reaction Package

- Sorption
  - Linear, equilibrium sorption
  - Nonlinear, equilibrium sorption
  - Linear, nonequilibrium sorption
  - Dual-domain mass transfer without sorption
  - Dual-domain mass transfer with sorption
- 1st-order kinetic reactions
  - radioactive decay or biodegradation
- Third-party add-on packages

Chemical Reaction Package

- Specification of reaction constants
  - Layer by layer:

    one value per layer or one 1D array for all layers
  - Cell-by-cell:

    one value per cell or one 2D array for each layer

Chemical Reaction Package

- The units for sorption constants must be such that the resulting retardation factor, *R*, is dimensionless
- Linear sorption

$$R = 1 + \frac{\rho_b}{\theta} K_d$$

$$[K_d][\rho_b] = \text{dimensionless}$$

$$\therefore [K_d] = [\rho_b]^{-1}$$

Chemical Reaction Package

- Freundlich sorption

$$R = 1 + \frac{\rho_b}{\theta} a K_f C^{a-1}$$

$$[\frac{\rho_b}{\theta} a K_f C^{a-1}] = \text{dimensionless}$$

$$\therefore [K_f] = [\rho_b]^{-1} [C]^{1-a}$$

- Langmuir sorption

$$R = 1 + \frac{\rho_b}{\theta} \frac{K_l \bar{S}}{(1 + K_l C)^2}$$

$$\left[\frac{\rho_b}{\theta} \frac{K_l \bar{S}}{(1 + K_l C)^2} \right] = \text{dimensionless}$$

$$\therefore [K_l] = [C]^{-1} = [\rho_b]^{-1} [\bar{S}]^{-1}$$

GCG Solver Package

- GCG solver package is used to solve the matrix equations resulting from application of the implicit finite-difference method to the dispersion, reaction, sink/source terms, and optionally the advection term.
- Specify
  - Number of outer iterations (set to >1 only for simulations with nonlinear reactions)
  - Number of inner iterations (30~50)
  - Concentration error criterion (usually 10^{-4}~10^{-6})

CLASS EXERCISE
with
MT3DMS

Adds 1000mg/l to recharge of zone 2 (columns 5 & 6) & simulates 100 secs

Example FILES on class web page

VERY IMPORTANT MT3D IS BASED ON FIXED FORMATS

Use guidance from today's class notes
&
MT3D manuals (in doc directory for mt3d and link on class web page)

To set up your own scenario and follow the examples

Use GWChart to view C(t)
&
ModelViewer to view C Contours in space