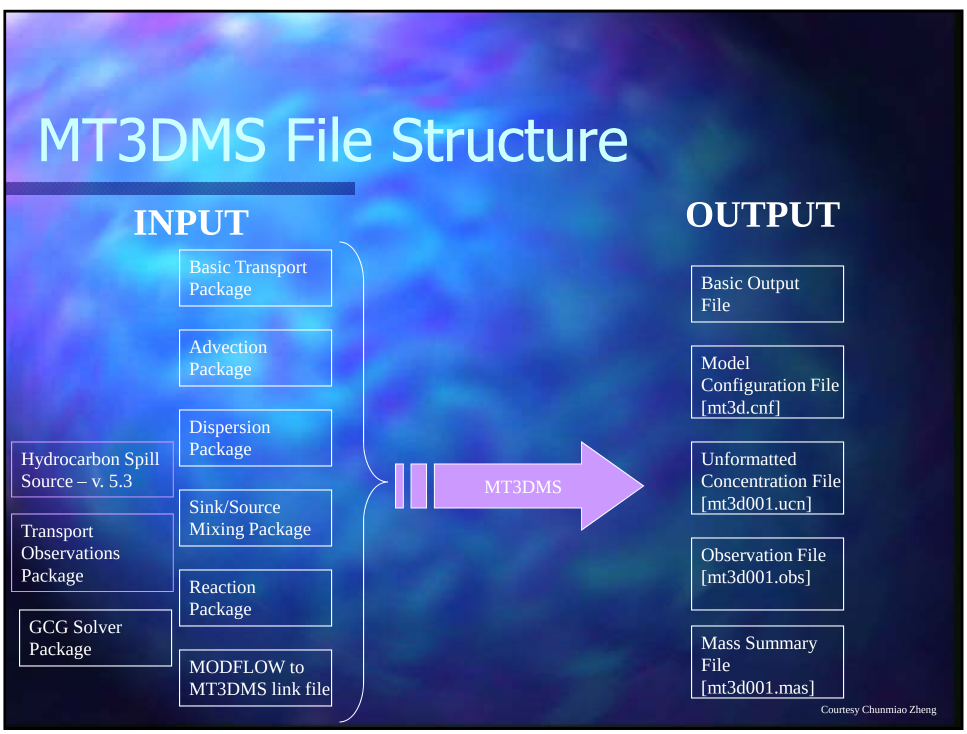

Presentation 8
MT3DMS—Packages


MT3DMS File Structure
INPUT
Basic Transport Package
Advection Package
Dispersion Package
Sink/Source Mixing Package
Reaction Package
MODFLOW to MT3DMS link file
Hydrocarbon Spill Source – v. 5.3
Transport Observations Package
GCG Solver Package
MT3DMS
OUTPUT
Basic Output File
Model Configuration File [mt3d.cnf]
Unformatted Concentration File [mt3d001.ucn]
Observation File [mt3d001.obs]
Mass Summary File [mt3d001.mas]
Courtesy Chunmiao Zheng

Measurement Units in MT3DMS

- Length and time units must be consistent with MODFLOW
- Concentration units are arbitrary as long as the following points are kept in mind:
  - Output concentration unit is the same as the input concentration unit
  - The mass budgets calculated by MT3DMS based on inconsistent concentration unit must be converted if absolute mass value is important
  - Consistent units must be used if nonlinear reaction is simulated

Courtesy Chunmiao Zheng

Linkage Between MODFLOW and MT3DMS

- Key assumption for standard MT3DMS applications: density change caused by solute transport is negligible
- The LMT Package: LMT is a MODFLOW package that saves advective velocities and source/sink flux information needed by MODFLOW
  - LMT saves information at the end of every MODFLOW timestep

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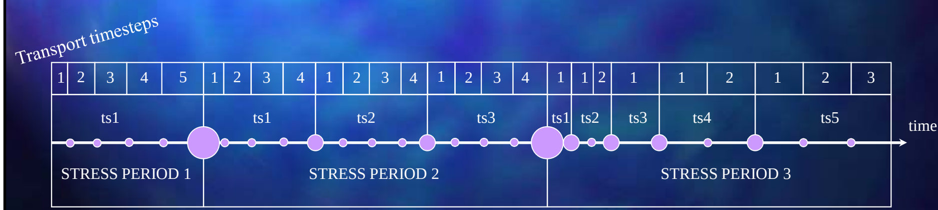
Temporal Discretization

- Stress periods
- Flow timesteps
- Transport timesteps



Steps for Running MT3DMS

- Run MODFLOW
  - Activate LMT to save flow information (not necessary for SEAWAT)
- Create MT3DMS input data files using text editor or preprocessor
- Run MT3DMS
- Post process

Courtesy Chunmiao Zheng

Typical Model Results of Interest

- Breakthrough concentration curves at specified observation points
- Plan or cross-sectional concentration contour maps

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MT3DMS Packages

- Basic Transport (BTN)
- Advection (ADV)
- Dispersion (DSP)
- Source-Sink Mixing (SSM)
- Chemical Reaction (RCT)
- Generalized Conjugate Gradient (GCG) Solver
- Transport Observations Package (TOB)
- Hydrocarbon Spill Source Package (HSS)

BTN Package

- Purpose: to specify
  - Basic information
  - Spatial discretization
  - Boundary and initial conditions
  - Printing and saving options
  - Temporal discretization

Courtesy Chunmiao Zheng

BTN Package (cont.)

- Model Layer Type (Laycon):
  - =0: confined layer
  - $\neq$ 0: unconfined or convertible
- Implications
  - LAYCON=0: user-specified DZ used as saturated thickness
  - LAYCON $\neq$ 0: MT3D determines saturated thickness internally (using MODFLOW approach)

Courtesy Chunmiao Zheng

BTN Package (cont.)

- HTOP: top elevation of 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

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BTN Package (cont.)

- IBOUND vs. ICBUND
  - Active cells in MODFLOW (IBOUND > 0) may be defined as inactive cells in MT3D
  - Inactive cells in MT3D – set ICBUND=0
  - IBOUND≠ICBUND to exclude active flow cells from transport calculations and speed up transport computation

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BTN Package (cont.)

- 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 timesteps in each stress period (NSTP), and the timestep multiplier (TSMULT) must be identical in flow and transport models

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Basic Transport (cont.)

- For each stress period
  - PERLEN (same as in MODFLOW)
  - NSTP (same as in MODFLOW)
  - TSMULT (same as in MODFLOW)
  - TSLNGTH(NSTP) (only for flow model other than MODFLOW)
  - DT0: maximum allowable transport stepsize
  - MXSTRN: maximum number of transport steps within one flow timestep
  - TTSMULT: transport stepsize multiplier within a flow-model timestep
  - TTSMAX: maximum transport stepsize within a flow model timestep (set to zero for no limit)

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ADV Package

- Purpose
  - To solve the advection components of the transport equation using one of the following options (through input variable `MIXELM`)
    - Finite Difference
      - Upstream weighting
      - Central-in-space weighting
    - Particle-Based Methods
      - MOC
      - MMOC
      - HMOC
    - TVD

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Selection of Solution for ADV

- Finite-Difference Method
  - Efficient and sufficiently accurate for problems with Pe < 2 to 4
  - For problems with Pe > 4, lead to numerical dispersion (upstream weighting) or artificial oscillation (central-in-space weighting)
  - Good option for initial test runs to make sure input/output all set properly; should produce negligible mass balance error (<0.1%)
- Particle Based Methods
  - For problems with Pe > 4 and relatively uniform grid
  - Select MOC for pure advection or strongly advection-dominated problems; otherwise, select HMOC
  - Mass balance error within 10%
- TVD
  - For problems with Pe > 4 and for which MOC/HMOC cannot produce satisfactory results (too large mass balance errors or too ‘rough’ breakthrough curves)

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ADV Package (cont.)

- Allowable stepsize 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:

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

  - MOC, MMOC, HMOC: $C_r \geq 1$ (generally set to 1.0)
  - Explicit Finite Difference, or TVD $C_r \leq 1$ (generally set between 0.5 and 1.0)

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ADV Package (cont.)

- In MT3DMS, a fully implicit finite-difference option 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.
- Only when the implicit finite-difference option is used for advection do the following two input variables take effect:
  - TTSMULT: transport stepsize multiplier
  - TTSMAX: maximum transport stepsize

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ADV Package (cont.)

- MOC
  - ITRACK =1 generally ok (1st order)
    =2 generally overkill (RK4)
    =3 suggested (combination)
  - WD $0.5 \le WD \le 1.0$
    = 0.5 generally ok
    =1.0 for purely advective transport
  - DCEPS $=10^{-5}$ generally ok
  - NPLANE =0 (random pattern) generally ok
    =1 for 2D plan
    =2 or 3: cross section or 3D
  - NPL =0 generally ok, may be as many as NPH
  - NPH ≤ 16 generally ok for 2D
  - NPMIN ≤ 32 generally ok for 3D
  - NPMAX set about 2 x NPH
  - SRMULT =1
- MMOC
  - INTERP =1 only option available
  - NLSINK =NPLANE generally ok
  - NPSINK =NPH generally ok
- HMOC
  - DCHMOC $=1\times10^{-3}$ generally ok

Courtesy Chunmiao Zheng

DSP Package

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

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

- Implicit scheme has no stepsize limitation

Courtesy Chunmiao Zheng

DSP Package (cont.)

- AL (longitudinal dispersivity, unit L)
  - Cell-by-cell
  - 2D array for each model layer
- TRPT (ratio of horizontal transverse dispersivity to longitudinal dispersivity)
  - One value per model layer
  - Input as 1D array for all layers
- TRPV
  - One value per model layer
  - Input as 1D array for all layers
- DMCOEF
  - One value per model layer
  - Input as 1D array for all layers
  - $D^*=\tau D_0$

Can now enter different DMCOEFF for each species (starting in version 5.2)

Courtesy Chunmiao Zheng

DSP Package (cont.)

- Literature review (see Zheng and Bennett, Chap. 9)
- Things to consider
  - More heterogeneity in flow model, smaller dispersivities in transport model
  - Scale dependent
  - Rule of thumb:
    - TRPT: 0.1 – 0.01
    - TRPV: 0.01 – 0.001
  - Temporal variations can account for significant amount of dispersion
  - Is dual domain more appropriate?

Courtesy Chunmiao Zheng

SSM Package

- Purpose: to solve the source and sink components of the transport equation
- With explicit finite difference method, subject to stepsize stability constraint

$$\Delta t_{SSM} = \min\left(\frac{R\theta}{q_s}\right)$$

Note: q_s is sink/source volumetric flow rate divided by cell volume

- Implicit scheme can be used to solve SSM component without stability constraint

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SSM Package (cont.)

- Specify hydraulic sinks/sources
  - Point sinks/sources
    - Constant-head cells (ITYPE=1)
    - Wells (ITYPE=2)
    - Drains (ITYPE=3)
    - Rivers (ITYPE=4)
    - General-head boundaries (ITYPE=5)
    - …
    - Mass loading (ITYPE=15)
  - Distributed sinks/sources
    - Recharge
    - Evapotranspiration

Courtesy Chunmiao Zheng

SSM Package (cont.)

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

Courtesy Chunmiao Zheng

SSM Package (cont.)

- Time-varying constant-concentration cell (ITYPE=-1)
  - This overrides 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})

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SSM Package (cont.)

- Specify concentrations of sinks/sources
  - 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
  - Sources
    - By default, concentration of all sources set equal to ZERO unless specified by user

Courtesy Chunmiao Zheng

SSM Package

- Constant-head vs. constant concentration
  - A constant-head cell in MODFLOW is treated as a regular fluid sink/source (like a well). The new 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 the aquifer
  - A constant-head cell can be specified as a constant-concentration if so desired

Courtesy Chunmiao Zheng

RCT Package

- Equilibrium-controlled linear and non-linear sorption
  - Linear Isotherm
  - Freundlich Non-Linear Isotherm
  - Langmuir Non-Linear Isotherm
- Non-equilibrium sorption
  - 1st order reversible kinetic reaction
- Linear Isotherm can be used to simulate thermal exchange between water and solid matrix (see Chapter 11 of v 5.3 manual)

RCT Package

- Radioactive decay or biodegradation
  - First-order irreversible rate reactions
- Dual-domain Mass Transfer
  - Advection dominated transport in fractures and/or high hydraulic conductivity zones (mobile domain)
  - Diffusion dominated in low hydraulic conductivity zones filled with immobile or relatively stagnant water (immobile domain)
- Zero-order reactions
  - Simulation of groundwater age and parameter sensitivities (v. 5.1)

GCG Solver Package

- Solve the linear equations resulting from the finite-difference formulation of
  - Dispersion, sink/source, and reaction terms
  - Advection term, if the finite-difference option is selected
- Control parameters
  - MXITER
  - ITER1
  - ISOLVE
  - NCRS
  - ACCL
  - CCLOSE
  - IPRGCG

Courtesy Chunmiao Zheng

TOBS Package

- Obtain the calculated concentration at an observation point that does not coincide with a model node
  - Observations at the closest node to observation point
  - Use bilinear interpolation to calculate results at the observation point

TOBS Package

- Save the calculated mass fluxes at any sink/source location
  - Individual sink/source location
  - Arbitrary group of sink/source cells (mass flux object)
- Calculate residuals errors at observation locations
  - Observations can be weighted
  - Residuals can be calculated for multiple times – at times closest to specified time or at specific time using TIMPRS in BTN

HSS Package

- Use to simulate the vertical migration of a light non-aqueous phase liquid (LNAPL) contaminant through the unsaturated zone and the formation of an oil lens on the water table
- Determines the rate of contaminant mass flux dissolved from the LNAPL to the groundwater

HSS Package

- Application of HSS Package to other problems:
  - Use to specify an arbitrary time varying mass loading source or boundary condition
  - Can be used to simulate any MT3D time-varying mass loading sources or boundary conditions

HSS Package

- Application of HSS Package to other problems (cont.):
  - Prior to v. 5.3, temporal variation of sources and boundary conditions had to be discretized into stress periods defining
  - HSS reduces the need to define stress periods to represent temporal variation of sources and boundary conditions