2D Transport Tutorial Part 3: MOC Solver Setup and Optimization

1. Background and Objectives

Recap

This document extends the previous stages of the 2D Transport Tutorial:

- In **2D Transport Step 01**, a steady-state flow model was constructed.
- In **2D Transport Step 02**, a transport model was configured and executed using the Standard Finite Difference (FD) solver.

Objective

This tutorial focuses on configuring and optimizing the Method of Characteristics (MOC) solver in MT3DMS. The goal is to analyze its behavior through targeted parameter tuning and compare the resulting concentration profiles with analytical benchmarks.

Core Considerations

- The MOC solver is particularly suited for reducing numerical dispersion. By setting longitudinal dispersivity to zero, both numerical and physical dispersion are effectively eliminated.
- When the solver type is changed (e.g., FD to MOC or MOC to MMOC), the flow model must be re-executed to regenerate the Flow Transport Link (FTL) file. However, when only internal parameters of a solver are modified, it is sufficient to re-run the transport model alone.

To examine the isolated effect of solver parameters, dispersion was initially disabled by setting the longitudinal dispersivity to zero. This established a controlled baseline. Once a stable and representative solution was obtained under these conditions, dispersion was subsequently reintroduced for comparative analysis.

The following key parameters were adjusted during the optimization of the MOC solver:

- number of initial particles per cell.
- maximum number of total moving particles.
- maximum number of moving particles per cell .

Discussion Prompts

- What physical and numerical mechanisms shape the breakthrough curve?
- How does increasing particle count per cell influence transport resolution?
- What role does the total particle cap play in maintaining computational accuracy?
- Why is it beneficial to increase the per-cell particle threshold in Advection2?

Reflection Questions

- Explain the shape of the concentration curve. What factors influence it?
- How does increasing the number of initial particles per cell help in refining MOC?
- What is the role of the total maximum number of moving particles?
- Why was the maximum particles per cell increased in Advection2 settings?

2. Changing the Solver to MOC

- Navigate to `Model > MODFLOW Packages and Programs > Groundwater Transport > MT3DMS or MT3D-USGS > ADV`.
- In the `Advection1` section,
  - change the `Advection Solution Scheme` to `Method of Characteristics (MOC)`.
- Click `OK` to apply the changes.

Running MODFLOW

- Click the green triangle below the `Grid` icon.
- Save the model in the directory `Coarse/coarse_MOC/` as `coarse.nam`.
- Confirm and execute the simulation.

Running MT3DMS

- Click the dropdown arrow next to the green triangle.
- Select `Export MT3D Input Files`.
- Save the input in `Coarse/coarse_MOC/` as `coarse.mtnam`.

Checklist:

- Verify the percent discrepancy reported in the `.lst` file.
- Record the simulation runtime for future comparison.

Visualizing the Results

1. Click Import and display result (the colored icon adjacent to the simulation run button).
2. Navigate to Coarse_MOC/ and select the relevant .ucn file.
3. Choose the final transport step (typically the last time step).
4. In the Select Model Results to Import window:
    - Classification will default to Model Result, and the Prefix input field will be inactive.
    - Change Classification to User Define.
    - The prefix field will now be editable; enter: Coarse_MOC.

Comparing Against Analytical Solution

- Open the .MTO file in Coarse_MOC/ and copy its contents.
- Launch the Excel analysis sheet and go to the Coarse worksheet.
- Paste the data and examine the overlaid plots of the numerical and analytical solutions across all observation points.

3. Optimizing the MOC Solver

Iteration 1: Increasing Particle Settings

- Navigate to Model > MODFLOW Packages and Programs > Groundwater Transport > MT3DMS or MT3D-USGS > ADV.
- In Advection1:
    - Increase Initial particles per cell (DCEPS (NPH)) from 10 to 16.
    - Raise Maximum total moving particles (MXPART) from 75,000 to 250,000.
- In Advection2:
    - Increase Maximum particles per cell (NPMAX) from 20 to 200.
- Click OK to save changes.

Note: Since the solver has not changed, re-running the flow model is not necessary. Only the transport model needs to be re-executed.

Repeat the steps in **Running MT3DMS**, **Visualizing the Results**, and **Comparing Against Analytical Solution**.

Iteration 2: Disabling Dispersion

- Go to `Data > Edit Data Sets > Required`.
- Expand `MT3DMS`, `MT3D-USGS`, or `GWT`.
- Locate `Longitudinal Dispersivity` and set it to `0`.

Repeat the steps in **Running MT3DMS**, **Visualizing the Results**, and **Comparing Against Analytical Solution**.

Iteration 3: Further Increasing Particle Density

- Navigate again to `ADV > Advection1`.
- Increase `Initial particles per cell (DCEPS / NPH)` from 16 to 32.

Repeat the steps in **Running MT3DMS**, **Visualizing the Results**, and **Comparing Against Analytical Solution**.

Iteration 4: Re-enabling Dispersion

- Go to `Data > Edit Data Sets > Required`.
- Expand `MT3DMS`, `MT3D-USGS`, or `GWT`.
- Reset `Longitudinal Dispersivity` to `10`.

Repeat the steps in **Running MT3DMS**, **Visualizing the Results**, and **Comparing Against Analytical Solution**.

Press `Ctrl + S` to save the model.