# 2D Transport Tutorial Part 4: Grid Refinement

## 1. Introduction

In this part of the tutorial, we focus on refining the computational grid to better capture solute transport behavior in the region of interest. In earlier steps, we defined the source as a point object within a coarse grid composed of `100 m × 100 m` cells. While sufficient for a preliminary run, this setup showed noticeable deviations between the numerical and analytical solutions. To investigate the causes of this discrepancy—particularly the role of spatial resolution—we now introduce grid refinement. By refining the grid in the region where the plume spreads, we aim to improve the accuracy of the simulation.

We will perform grid refinement in the area where the plume spreads. This will involve the following key updates:

- **Refining the grid** by subdividing each row and column in the plume region.
- **Redefining the source** as a rectangular object that maintains the original physical dimensions (`100 m × 100 m`) but is now spread across multiple smaller cells.
- **Shifting the observation points** to preserve correct spacing from the new source boundary.

These changes ensure consistency with both the physical intent of the model and the expectations set by the analytical solution. Once updates are made, we will re-run the simulation and compare results with previous outputs.

## 2. Refining the Grid in ModelMuse

To improve spatial resolution in the region where the solute plume spreads, we will refine the grid by subdividing selected rows and columns

### Steps

1. Click on the `Subdivide Grid Cells` icon in the toolbar.
2. Using your cursor, select the area of the model where the plume is expected to spread—this corresponds to **rows 5 to 7** and **columns 3 to 25**.
3. A dialog box will appear with the following fields:

- "From Column": 3
  "Through Column": 25
  "Subdivide each column into": 1 (change this to 10)
- "From Row": 5
  "Through Row": 7
  "Subdivide each row into": 1 (change this to 10)

4. Click "OK" to apply the refinement.

The selected region is now refined to smaller cells of size 10 m × 10 m.

## 3. Redefining the Contaminant Source

1. Use the Create Rectangle Object tool (rectangle icon next to the Create Straight Line Object tool).
2. Draw a rectangle anywhere on the grid to activate the object.
3. Name the object source.
4. Open the object's Vertices tab and manually enter the following coordinates:
   - (300, -500)
   - (400, -500)
   - (400, -600)
   - (300, -600)
   - (300, -500) *(to close the rectangle)*
5. **Note:** In the video, the rectangle is initially drawn with incorrect coordinates. This is corrected later in the demonstration. Please use the coordinates listed above when defining the object in your model.
6. Go to MODFLOW Features > SSM, then configure the following:
   - Check Specified Concentration.
   - To enter values, double-click the relevant text fields. If the fields appear inactive, make sure the Number of times field (located in the lower-left corner of the dialog) is set to 1, not 0.
   - Starting Time: 0
   - Ending Time: 86,400,000
   - Chem concentration: 1
7. Click "OK" to apply the settings and close the dialog box.

## 4. Updating Observation Point Locations

With the refined grid and rectangular source in place, we must now adjust the observation point coordinates. Originally, the point source was placed at the center of a coarse grid cell. That center is now the center of the new rectangular source, which extends 50 meters to both the left and right, covering a total width of 100 meters.

- As a result, the **right edge of the rectangle**, located at $x = 400$, becomes the new reference for measuring observation distances.
- To preserve the original spacing from the source, each observation point's $x$-coordinate must be increased by 50 meters.
- No changes are required along the $y$-axis.

**Steps**

- **Obs100:** Change $x = 450$ to $x = 500$
- **Obs300:** Change $x = 650$ to $x = 700$
- **Obs500:** Change $x = 850$ to $x = 900$
- **Obs1000:** Change $x = 1350$ to $x = 1400$

For each point:

1. Click on the point object.
2. Go to the `Vertices` tab.
3. Edit the $x$-coordinate by adding 50.
4. Leave the $y$-coordinate unchanged.

## 5 Running Flow and Transport Models for Different Solvers

After refining the grid and updating the source and observation points, we now proceed to run the simulation using two different solvers: Standard Finite Difference (FD) and Method of Characteristics (MOC). Each run will be followed by post-processing to compare results with the analytical solution.

### Run 1: Standard Finite Difference (FD)

### Changing the Solver

- Navigate to `Model > MODFLOW Packages and Programs > Groundwater Transport > MT3DMS or MT3D-USGS > ADV`.
- In the `Advection1` section, set the `Advection Solution Scheme` to `Standard Finite Difference`.

### Running MODFLOW

- Click the green triangle below `Grid`.
- Navigate to `Fine/Fine_FD/`.
- Save the model as `Fine.nam`.
- Click `"OK"` to apply the changes and run the simulation.

### Running MT3DMS

- Click the dropdown next to the green triangle.
- Select `Export MT3D Input Files`.
- Name the file `Fine.mtnam`.
- Monitor the run using `ModelMonitor` and check the listing file for errors.
- Close the command window after the simulation completes.

### Visualizing the Results

1. Click `Import and display result` (colored icon next to the simulation run button).
2. Navigate to `Fine/Fine_FD/` and select the relevant `.ucn` file.
3. Select 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` field will be inactive.
    - Change `Classification` to `User Define`.
    - Enter the prefix: `Fine_FD`.

### Comparing Against Analytical Solution

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

### Run 2: Method of Characteristics (MOC)

#### Changing the Solver

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

#### Running MODFLOW

- Click the green triangle below `Grid`.
- Navigate to `Fine/Fine_MOC/`.
- Save the model as `Fine.nam`.
- Click `"OK"` to apply the changes and run the simulation.

#### Running MT3DMS

- Click the dropdown next to the green triangle.
- Select `Export MT3D Input Files`.
- Name the file `Fine.mtnam`.
- Monitor the run using `ModelMonitor` and check the listing file for errors.
- Close the command window after the simulation completes.

#### Visualizing the Results

1. Click `Import and display result` (colored icon next to the simulation run button).
2. Navigate to `Fine/Fine_MOC/` and select the relevant `.ucn` file.
3. Select 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` field will be inactive.
    - Change `Classification` to `User Define`.
    - Enter the prefix: `Fine_MOC`.

### Comparing Against Analytical Solution

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

## 6. Breakthrough Curve Comparison (Refined Model)

As in the previous tutorial, we conclude this exercise by comparing breakthrough curves derived from the numerical model and the analytical solution. While the process remains the same, the purpose here is distinct: to evaluate how grid refinement and solver selection affect the accuracy of simulated concentrations at key observation points.

### Steps

- In the Streamlit app, define observation points at the same distances from the updated source boundary.
- Download the resulting CSV containing analytical concentrations over time.
- Open the provided Excel sheet and paste this data into the designated section under the `Fine` worksheet.
- From your updated `.MTO` files (`Fine_FD/` and `Fine_MOC/`), copy the numerical breakthrough data and paste it into the same worksheet.