# 2D Transport Tutorial Part 5: Dirac Pulse Injection and Breakthrough Curve Analysis

## 1. Objective

In this tutorial, we simulate a Dirac pulse—a brief injection of solute mass over a short duration—and analyze its transport behavior using both Finite Difference (FD) and Method of Characteristics (MOC) solvers. The results will be compared against an analytical solution generated through a specialized Streamlit application.

## 2. Saving a New Model Version

Begin by saving your current refined model in a new folder to preserve the previous configuration.

- Choose a new working directory (e.g., `Dirac_FD/`).
- Save the model under an appropriate name (e.g., `Dirac.nam`).

## 3. Configuring Flow Model Time Discretization

- Go to `Model > MODFLOW Time`
- In the bottom-left corner of the dialog, set `Number of Stress Periods` to `3`.
- Set the following parameters:
  - **Period 1 (Steady-State):**
    - `Starting Time: -1`
    - `Ending Time: 0`
    - `Maximum first time step length: 1`
    - `Multiplier: 1`
  - **Period 2 (Injection):**
    - `Starting Time: 0`
    - `Ending Time: 10`
    - `Maximum first time step length: 10`

    - Multiplier: 1
  - **Period 3 (Transport):**
    - Starting Time: 10
    - Ending Time: 4320000
    - Maximum first time step length: 7200
    - Multiplier: 1.2
- Click "OK".

## 4. Configuring Transport Model Time Discretization

- Go to Model > MODFLOW Time
- Choose MT3DMS or MT3D-USGS
- In the bottom-left corner of the dialog, set Number of MT3DMS Periods to 3.
- Set the following parameters:
  - **Period 1 (Steady-State):**
    - Starting Time: -1
    - Ending Time: 0
    - Initial Time Step: 86400
    - Max Transport Steps per Flow Step: 1000
    - Time Step Multiplier: 1
    - Maximum Step Size: 0
  - **Period 2 (Injection):**
    - Starting Time: 0
    - Ending Time: 10
    - Initial Time Step: 10
    - Max Transport Steps per Flow Step: 1000
    - Time Step Multiplier: 1
    - Maximum Step Size: 0
  - **Period 3 (Transport):**
    - Starting Time: 10
    - Ending Time: 4320000
    - Initial Time Step: 7200
    - Max Transport Steps per Flow Step: 1000
    - Time Step Multiplier: 1
    - Maximum Step Size: 0
- Click "OK".

## 5. Updating Transport Parameters

Since the transport distance is now much shorter (30–100 m), set:

- Longitudinal dispersivity $\alpha_L = 5$ m (Thumb rule: $\alpha_L \approx 10\%$ of travel distance)

## 6. Adapting Boundary Conditions

- Select the constant head objects on the inlet and outlet boundaries.
- Edit the `CHD` time periods to start at $-1$ s and end at 432000 s.

## 7. Defining Injection Source

### Activating relevant package

- Go to `Model > MODFLOW Packages and Programs > Boundary Condition (Expand) > Specified Flux`.
- Check the box next to `Well`.
- Go to `Model > MODFLOW Packages and Programs > Post Processors (Expand)`.
- Uncheck the box next to `MODPATH` to deactivate it.

### Defining the Injection Point

- Select `Create point object`.
- Click anywhere on the grid to place the object.
- Name the object `solute_injection`.
- Go to the `Vertices` tab.
- Enter: `X = 400`, `Y = -550`
- Go to `MODFLOW Features Tab check the box next to Well`, and do the following:
  - Set `Number of times: 3`
  - Enter the following injection schedule:

| Starting Time | Ending Time | Pumping Rate ($m^3$/s) |
|---|---|---|
| $-1$ | 0 | 0 |
| 0 | 10 | 0.001 |
| 10 | 4320000 | 0 |

- In the same tab, check the box next to `SSM`.

- Set `Number of times: 3`
- Enter the concentration loading as follows:

| Starting Time | Ending Time | Concentration (mg/L) |
|---|---|---|
| $-1$ | 0 | 0 |
| 0 | 10 | 100000 |
| 10 | 4320000 | 0 |

- Click `"OK"` to close the dialog.

## 8. Placing Observation Points

Insert a new point object at a distance of 30 m downstream:

- Location: $(x = 430, y = -550)$
- Name the object `Obs30`
- Under: `Data Sets> Required>MT3DMS or MT3d-USGS` ,
- enable `MT3DMS_Observation_Location > True`

## 9. Selecting the solver

Set advection scheme to `Standard Finite Difference`
navigate to:
`Model > MODFLOW Packages and Programs > Groundwater transport (Expand) > MT3DMS or MT3D-USGS` then `Advection 1 > Advection Solution Scheme > Standard Finite Difference`

## 10. Running MODFLOW

- Click the green triangle below `Grid`
- Navigate to `Dirac/Dirac_FD/`
- Save as `Dirac.nam`
- Run the simulation

## 11. Running MT3DMS

- Click the dropdown next to the green triangle
- Click `Export MT3D Input Files`
- Name the file `Dirac.mtnam`

- Check `ModelMonitor` and the listing file
- Close the command window

## 12. Visualize and Export Results

- Load the final `.UCN` file.
- Observe the concentration pulse movement through the grid.
- Open the `.MTO` file and copy the data into the `Dirac` worksheet of the Excel template.
- Review the breakthrough curve under the FD configuration.

## 13. Run with Method of Characteristics (MOC)

Repeat the same process using the MOC solver:

- Change the advection method to `MOC`.
- Save the model in `Dirac_MOC/` and run the flow simulation.
- Run MT3DMS and monitor mass balance in the listing file.
- Load the updated `.UCN` results and paste the `.MTO` data into the Excel sheet.
- Observe the breakthrough curve. MOC results typically show sharper transitions and minor oscillations.

## 14. Analytical Comparison with Streamlit App

- Open the **2D Dirac Streamlit App**.
- Enter the following parameters in the Streamlit app:
  - `Released Mass: 1000 g`
  - `Specific Discharge: 0.432 m/d`
  - Toggle the switch for `Source equivalent to model cell` to account for 10 m aquifer thickness.
  - `Longitudinal Dispersivity: 5 m`
  - Set breakthrough curve extraction at 30 m.
  - Set maximum time = 100 days, and concentration range = 1 g/m$^3$.
- Download the CSV and paste into the same Excel sheet under `Dirac`.

### Interpretation

Compare the analytical breakthrough curve with both FD and MOC results:

- MOC shows excellent agreement with the analytical solution.
- FD displays significant numerical dispersion, resulting in a smeared response.

## 15. Summary

In this tutorial, we simulated a Dirac pulse injection scenario and examined solute transport using both FD and MOC methods. The breakthrough curve analysis confirmed that:

- The MOC solver accurately captures the sharp pulse shape.
- FD suffers from numerical dispersion under such conditions.

The analytical comparison highlights the importance of solver selection and temporal configuration when modeling short-duration events.