

```

1 # Grid parameters
2 grid:
3   # Number of cells [Nx, Ny, Nz]
4   dimension: [170, 150, 1]
5   # Size of each cell [dx, dy, dz]
6   cell size: [1.0, 1.0, 1.0]
7
8 # Physics parameters
9 physics:
10 porosity: 0.2
11 molecular diffusion: 0.00000060 #m^2/min
12 longitudinal dispersivity: 0.01
13 transverse dispersivity: 0.001
14 velocity:
15   # Type of the file imported (e.g., modflow)
16   type: modflow
17   # Path to the file (e.g, .ftl file generated by the
18   # LMT Modflow package)
19   file: tmp/model-{}.ftl
20
21 # Simulation parameters
22 simulation:
23   particles:
24     # Number of particles
25     N: 100000
26     # Define the volume where
27     # p1x <= x <= p2x
28     # p1y <= y <= p2y
29     # p1z <= z <= p2z
30     start:
31       # Point 1 [p1x, p1y, p1z]
32       p1: [25, 65, 0]
33       # Point 2 [p2x, p2y, p2z]
34       p2: [37, 85, 1]
35
36     # Time step #days
37     dt: 0.05
38     # Number of steps
39     steps: 100000
40

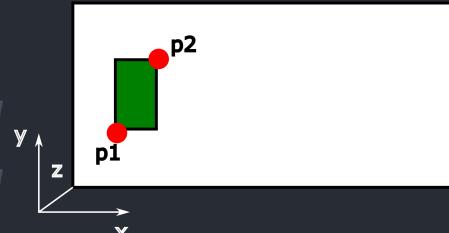
```

here you need to define the grid parameters of your model

here you need to define the physics parameters and indicate which is the velocity field that has to be used in the transport simulation. Following the structure of this Jupyter Notebook, the flow field is generated by MODFLOW and the file containing the data is in the tmp folder. The "{}" is going to be replaced by the Monte Carlo iteration number.

here you need to define the simulation parameters. Since we are working with a Lagrangian model, the contaminant plume is discretized into particles. The number of particles has to be chosen such that if increased, the result of the simulation doesn't change. This is a variable that needs to be tested with a single scenario, before implementing the full Monte Carlo analysis.

In this section you need also to define the initial position of the contaminant plume:



this is also the section where you need to define the time discretization and the number of steps of the simulation.

here you need to define where you want your simulation results to be saved, and to what they are related. As written in the Jupiter Notebook, the output is a .csv file that contains the data related to the cbt curves at selected control planes (items). Here the simulations results are saved in the result-{}.csv file, where the {} is replaced with the Monte Carlo iteration number. NB, you can add as many items you need, just coping and pasting from line 52 to line 57 and changing the position of the evaluated control plane.

```

41 # Output parameters
42 output:
43   # csv file containing post-proc
44   csv:
45     # Path to the file, The '{}'
46     # Monte Carlo iteration num
47     file: output/result-{}.csv
48     # Data is computed every 'skip' steps
49     skip: 1
50     # List of items to be computed. You can add any number of items
51     items:
52       - label: cbtx x=117.0
53         # Compute fraction of particles that have crossed a plane
54         # Located at x=117.0
55         type: after-x
56         x: 117.0
57
58       - label: cbtx x=168.0
59         # Compute fraction of particles that have crossed a plane
60         # located at x=168.0
61         type: after-x
62         x: 168.0
63
64     # Export snapshots (optional)
65     snapshot:
66       # Path to the file. The '*' is
67       # step number. A file is generated
68       # Note that exporting a large number of snapshots may slow down the simulation.
69       file: output/snap-{}-* .csv
70       # List of time steps
71       # steps: [0, 50000, 100000]
72       # Instead of 'steps', it is possible to use 'skip' as for
73       # the csv file, for example:
74       skip: 400
75
76

```

here you can ask to generate the snap-{}-* .csv file which contains the particles positions (in which the plume has been discretized into) at the selected time step. To do that, you can define the time steps that you are interested in, or (if they are many) you can define the interval (skip) between them. In the name of the file: **Evaluated Time Step**

snap-{}-* .CSV

Monte Carlo Iteration