pyDiffusionFDM Testing

John P. Ortiz

September 24, 2024

1 diffusionCoupon

Consider a situation where the boundary $x = 0$ is held at a constant concentration (for instance one face of a soil or rock sample is exposed to a tank with fixed concentration of solute). This is a commonly used experimental method (sometimes referred to as "diffusion coupon experiment") for determining diffusivities in rocks and soils. Suppose the concentration of solute in the sample is initially zero, and assuming that the sample extends for a "relatively long" distance, so that it is practically "semi-infinite" along x (see Figure 1).

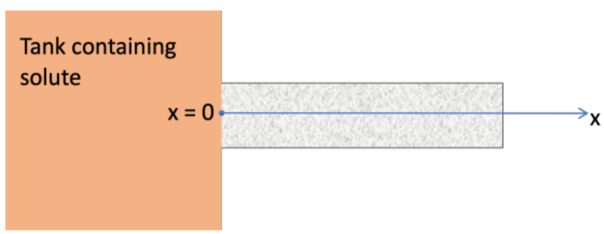

Figure 1: Schematic of the semi-infinite "diffusion coupon" experiment."

The diffusion equation and boundary conditions are:

$$\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} = 0 \tag{1}$$

In a true "diffusion coupon", the boundary conditions are:

$$C(0,t) = C_0; C(x,t) \to 0 \text{ as } x \to \infty \tag{2}$$

which is generally a good approximation as long as the length of the column is sufficiently greater than the characteristic length of diffusion.

If this is not the case and a finite domain is needed, the following boundary conditions can be used in the model:

$$C(0,t) = C_0; -D\frac{\partial C}{\partial x} = 0 \text{ on } x = L \tag{3}$$

such that there is a no-flux (2nd-type, Neumann) BC on the boundary $x = L$. This can be modeled as a finite domain using a summation of fundamental diffusion equation solutions using image sources to represent the no-flux BC on the boundary. We therefore compare the pyDiffusionFDM model to results from both the semi-infinite domain and the finite domain analytical solutions.

1.1 Analytical Solutions

For the semi-infinite domain case, the analytical solution is as follows:

$$C(x,t) = C_0 \mathrm{erfc}\left(\frac{x}{2\sqrt{Dt}}\right) \tag{4}$$

For the finite domain case, the analytical solution can be constructed as follows:

$$C(x,t) = C_0 - 4\sum_{k=1}^{\infty}\left[\sin\left(2k+1)\pi\frac{x}{2L}\right)\cdot \exp -\frac{(2k+1)^2\pi^2 Dt}{4L^2(2k+1)\pi}\right] \tag{5}$$

1.2 Input File

```
# INPUT FILE FOR FDM DIFFUSION MODEL
#---------------------------------------------------------------
# Model Parameters
#---------------------------------------------------------------
outfilePrefix: ''   #[str] name to prefix all generated output files
# TIME PARAMETERS
dt: 10.              #[s] time discretization
t_initial: 0.       #[s] (default 0)
t_final: 36000.      #[s]

# DOMAIN PARAMETERS
L: 0.5              #[m] domain length
dx: 0.05             #[m] spatial discretization

# TRANSPORT PARAMETERS
D: 1.e-5             #[m^2/s] tracer diffusion coefficient (1.e-5)
phi: 1.0            #[-] porosity (1.0 = no rock)
# A: 0.003167         #[m^2] cross-sectional area
# rho_b: 2.57e3       #[kg/m^3]

# INITIAL CONDITIONS
initial_conditions:
    all: 0.0            #[Mass_tracer/Mass_fluid] inital concentration everywhere
    left: 1.00             # initial concentration left  boundary (x=0.)
    right: 0.00           # initial concentration right boundary (x=x_max.)
```

```
# BOUNDARY CONDITIONS
# [[ bc_types Array ]]
#     bc_type: 1 --> 1st-type (Dirichlet)
#     bc_type: 2 --> 2nd-type (Neumann)
bc_types: [ 1, 2 ]

# [[ bc_values Array ]]
bc_values: [ 1.00, 0. ]
```

1.3 Results

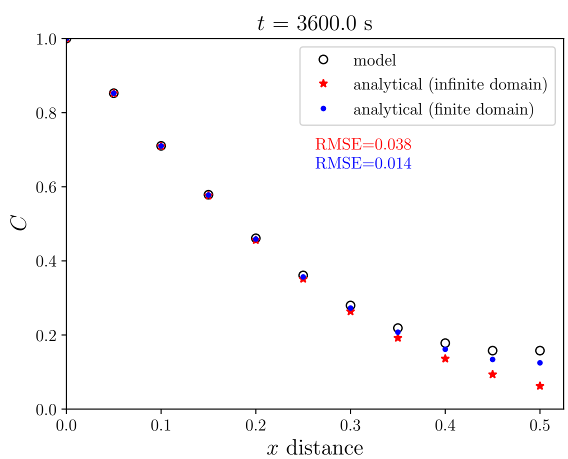

Figure 2: Comparison of concentration profiles to two analytical solutions, one with semi-infinite domain and one with a finite domain using a summation of image sources.

Add more info later...

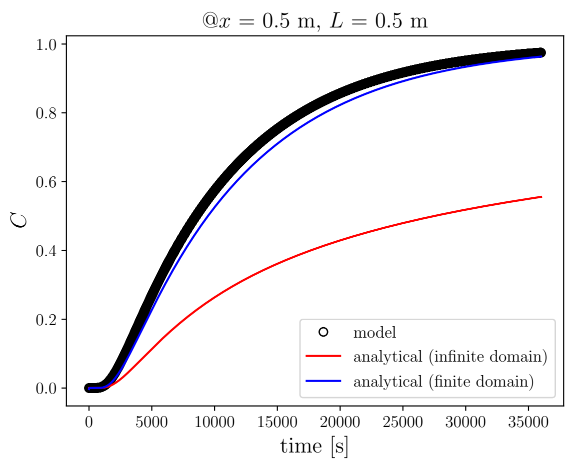

Figure 3: Comparison of breakthrough curves to two analytical solutions, one with semi-infinite domain and one with a finite domain using a summation of image sources.

2 transientDirichlet

This test simulates the 1-D diffusion coupon experiment, but with an arbitrary time-varying Dirichlet boundary condition on $x = 0$. The file for the BC is shown in subsection 2.2.

2.1 Input File

```
# INPUT FILE FOR FDM DIFFUSION MODEL
#---------------------------------------------------------------
# Model Parameters
#---------------------------------------------------------------
outfilePrefix: ''   #[str] name to prefix all generated output files
# TIME PARAMETERS
dt: 10.              #[s] time discretization
t_initial: 0.       #[s] (default 0)
t_final: 36000.      #[s]

# DOMAIN PARAMETERS
L: 0.5              #[m] domain length
dx: 0.05             #[m] spatial discretization

# TRANSPORT PARAMETERS
D: 1.e-5             #[m^2/s] tracer diffusion coefficient (1.e-5)
phi: 1.0            #[-] porosity (1.0 = no rock)
# A: 0.003167         #[m^2] cross-sectional area
# rho_b: 2.57e3       #[kg/m^3]

# INITIAL CONDITIONS
initial_conditions:
    all: 0.0            #[Mass_tracer/Mass_fluid] inital concentration everywhere
    left: 1.00             # initial concentration left  boundary (x=0.)
    right: 0.00           # initial concentration right boundary (x=x_max.)

# BOUNDARY CONDITIONS
# [[ bc_types Array ]]
#     bc_type: 1 --> 1st-type (Dirichlet)
#     bc_type: 2 --> 2nd-type (Neumann)
bc_types: [ 1, 2 ]

# [[ bc_values Array ]]
bc_values: [ 'inletDirichletBC.csv', 0. ]
```

2.2 BC File

```
time,C
0.0,1.0
125.,0.85
500.,0.83
1000.,0.80
2000.,0.75
3000.,0.70
7000.,0.82
9000.,0.87
12000.,0.90
15000.,0.80
17000.,0.70
20000.,0.60
25000.,0.4
30000.,0.25
36000.,0.2
```

2.3 Results

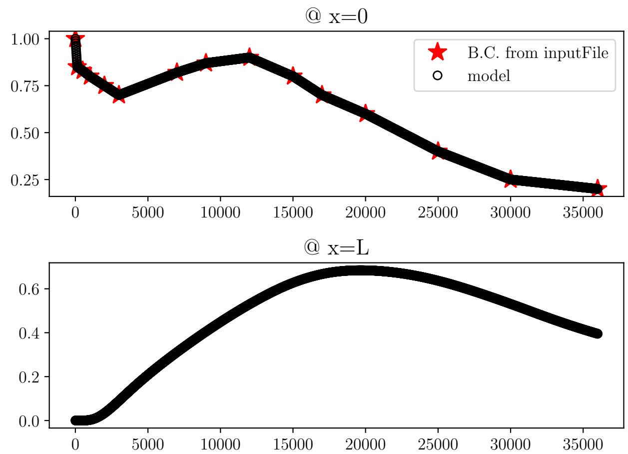

Figure 4: Comparison of simulated values with the transient Dirichlet BC plotted for reference.