pyDiffusionFDM Testing

John P. Ortiz

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1 diffusionCoupon

This test simulates a 1-D diffusion coupon experiment.
Dirichlet B.C. at x=0
Neumann (no-flux) B.C. at x=L.

1.1 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: [ 1.00, 0. ]
```

1.2 Results

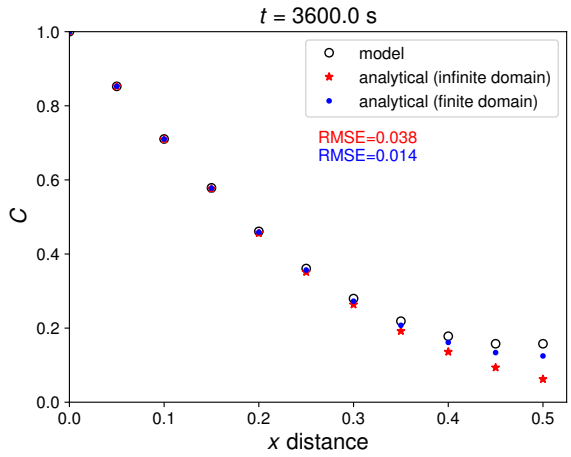

Figure 1: Comparison of concentration profiles to two analytical solutions, one with semi-infinite domain and one with a finite domain using a summation of image sources.

Add more info later...

2 transientDirichlet

This test simulates a 1-D diffusion coupon experiment with a time-varying Dirichlet Boundary condition on x=0.

Neumann (no-flux) B.C. at x=L.

2.1 Input File

```
# INPUT FILE FOR FDM DIFFUSION MODEL
#-----------------------------------------------------------------
# Model Parameters
```

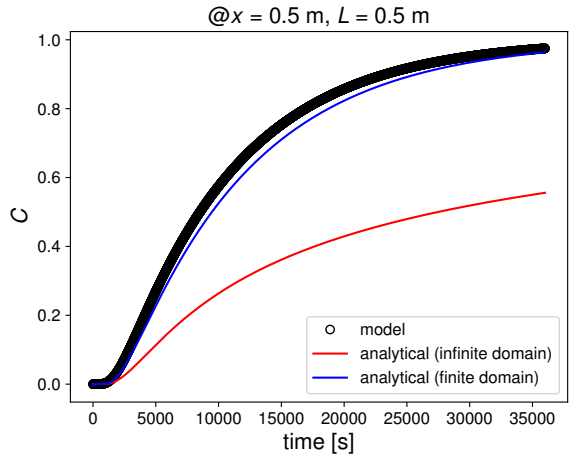

Figure 2: Comparison of breakthrough curves to two analytical solutions, one with semi-infinite domain and one with a finite domain using a summation of image sources.

```
#-----------------------------------------------------------------
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 Results

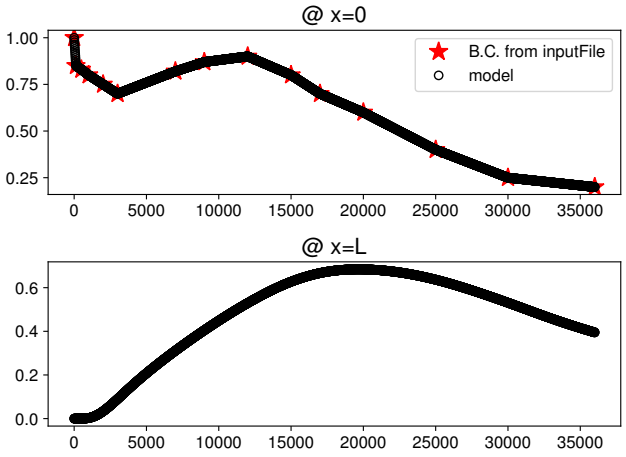

Figure 3: Plot.