pulse2d_simplemodel

March 22, 2019

1 Writing a simple model

1.1 Part 1: Simple model development

1.1.1 Objective: Read model input files, calculate output over model domain, write model output files

This model is based on Example 6.2 of Bedient et. al (1999):

A tank holding chloride at a concentration of 10,000 mg/L accidentally leaks over an area of 10 m^2 into an aquifer. Assume the chloride is a completely conservative tracer, that D_x = 1 m^2/day and D_y = 0.1 m^2/day, and that the seepage velocity (V_w) is 1 m/day.

For our model, we're going to define a domain of 5-100 m from the leak at 5 m intervals. For each interval in our domain we will calculate:

- a) The time required to reach the interval node

$$t = \frac{R_t x}{V_w}$$

where R_t is the retardation with time, x is the distance from leak source, and V_w is the seepage velocity. * b) Peak concentration

$$C_{max} = \frac{C_0 A}{4t\pi(D_x D_y)^{1/2}}$$

where C_0 is the initial chloride concentration, A is the spill area, t is the time for the plume to reach the interval node, and D_x and D_y are the dispersion cefficients in the x and y directions, respectively. * c) Plume Dimensions

$$3\sigma_x = 3(2D_x t)^{1/2}$$

$$3\sigma_y = 3(2D_y t)^{1/2}$$

where $3\sigma_x$ and $3\sigma_y$ are the plume dimensions in the x and y directions within three standard deviations from the mean (99.7% containment), respectively.

Implementation algorithm: 1. Define functions to calculate equations for parts a, b, and c. 2. Read in input parameters from *pulse2D_input.txt* and define input variables 4. Define model domain and interval size 5. Define vectors to store output data 6. Write for loop to iterate over model domain 7. Apply functions for a, b, and c for each interation and store values 9. Write output file 8. Plot data

References Bedient, P.B., Rifai, H.S., and Newell, C.J. (1999). Ground water contamination: Transport and remediation (2nd edition). ISBN: 0-13-013840-1.

```
In [1]: # IMPORT PACKAGES
        import math  # functions like sqrt and pi are parth of the math package
        import re  # regular expressions
        import numpy as np  # linearly spaced vector

        # plotting
        from matplotlib import rcParams  # next 3 lines set font family for plotting
        rcParams['font.family'] = ['serif']
        rcParams['font.sans-serif'] = ['Optima']
        rcParams['font.serif'] = ['Didot']
        import matplotlib.pyplot as plt
        plt.rcParams.update({'font.size': 18})

In [2]: # STEP 1: FUNCTIONS
        # custom functions always go at the very type of your code - you can't use them until yo

        # PART A:
        def time2node(x,Rt,Vw):
            t = (Rt*x)/Vw
            return t

        # PART B:
        def peakC(t,C0,A,Dx,Dy):
            Cmax = (C0*A)/(4*t*math.pi*math.sqrt(Dx*Dy))
            return Cmax

        # PART C:
        def plumeDim(t,D):
            sigma3 = 3*math.sqrt(2*D*t)
            return sigma3

In [3]: # STEP 2: Read in input parameters from *pulse2D_input.txt* and define input variables
        header_str = '^#'  # character to define header string in input file
        #var_strs = ['Dx','Dy','Vw','C0','A','Rt']  # variable names to search for

        # initialize variables - variables created within a for loop won't exist after the final
        Dx = 0
        Dy = 0
        Vw = 0
        C0 = 0
        A = 0
        Rt = 0

        f = open('pulse2D_input.txt')
        print('LINES----------')
        for line in f.readlines():
            header = re.search(header_str,line)
            if header is None:
```

```python
            lst = re.split('\t',line)
            print(lst)
            Dx_re = re.search('^Dx',line)
            Dy_re = re.search('^Dy',line)
            Vw_re = re.search('^Vw',line)
            CO_re = re.search('^CO',line)
            A_re = re.search('^A',line)
            Rt_re = re.search('^Rt',line)

            if Dx_re is not None:
                Dx = float(lst[1])
            if Dy_re is not None:
                Dy = float(lst[1])
            if Vw_re is not None:
                Vw = float(lst[1])
            if CO_re is not None:
                CO = float(lst[1])
            if A_re is not None:
                A = float(lst[1])
            if Rt_re is not None:
                Rt = float(lst[1])


    f.close()
    print('\nVARIABLES---------')
    print(Dx)
    print(Dy)
    print(Vw)
    print(CO)
    print(A)
    print(Rt)

    # STEP 3: Define model domain and interval size
    h = 5
    domain = np.linspace(5,100,20)
    print('\nDOMAIN NODES----------')
    print(domain)
```

```
LINES----------
['PARAMETER', 'VALUE\n']
['Dx', '1.000000\n']
['Dy', '.1000000\n']
['Vw', '1.000000\n']
['CO', '10000.00\n']
['A', '10.00000\n']
['Rt', '1.000000\n']

VARIABLES---------
```

```
1.0
0.1
1.0
10000.0
10.0
1.0

DOMAIN NODES----------
[  5.  10.  15.  20.  25.  30.  35.  40.  45.  50.  55.  60.  65.  70.
  75.  80.  85.  90.  95. 100.]
```

In [4]:
```python
# STEP 4: Define vectors to store output data
t_out = []
Cmax_out = []
sigma3x_out = []
sigma3y_out = []

# STEP 5: Write for loop to iterate over model domain
for x in domain:

    # STEP 6: Apply functions for a, b, and c for each interation and store values
    t = time2node(x,Rt,Vw)  # calculate value
    t_out.append(t)  # store value
    Cmax = peakC(t,C0,A,Dx,Dy)
    Cmax_out.append(Cmax)
    sigma3x = plumeDim(t,Dx)
    sigma3x_out.append(sigma3x)
    sigma3y = plumeDim(t,Dy)
    sigma3y_out.append(sigma3y)

print('OUTPUT: t')
print(t_out)
print('\nOUTPUT: Cmax')
print(Cmax_out)
print('\nPLUME DIMENSIONS:----')
print('\nsigma3x')
print(sigma3x_out)
print('\nsigma3y')
print(sigma3y_out)
```

```
OUTPUT: t
[5.0, 10.0, 15.0, 20.0, 25.0, 30.0, 35.0, 40.0, 45.0, 50.0, 55.0, 60.0, 65.0, 70.0, 75.0, 80.0,

OUTPUT: Cmax
[5032.921210448703, 2516.4606052243516, 1677.6404034829013, 1258.2303026121758, 1006.58424208974

PLUME DIMENSIONS:----
```

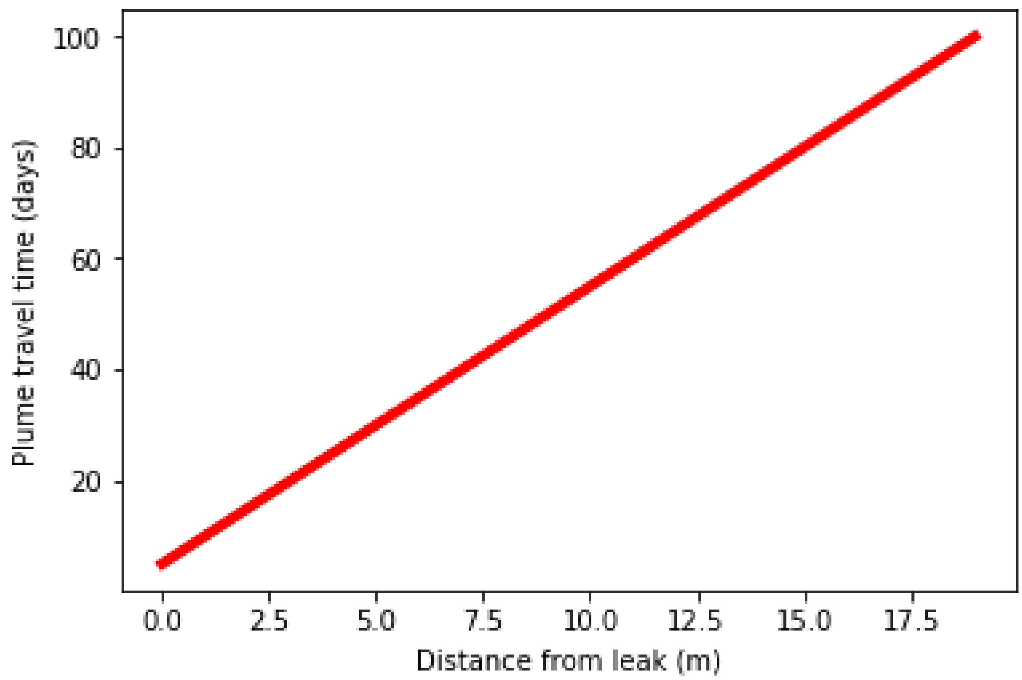
```
sigma3x
[9.486832980505138, 13.416407864998739, 16.431676725154983, 18.973665961010276, 21.2132034355964

sigma3y
[3.0, 4.242640687119286, 5.196152422706632, 6.0, 6.708203932499369, 7.348469228349534, 7.9372539
```

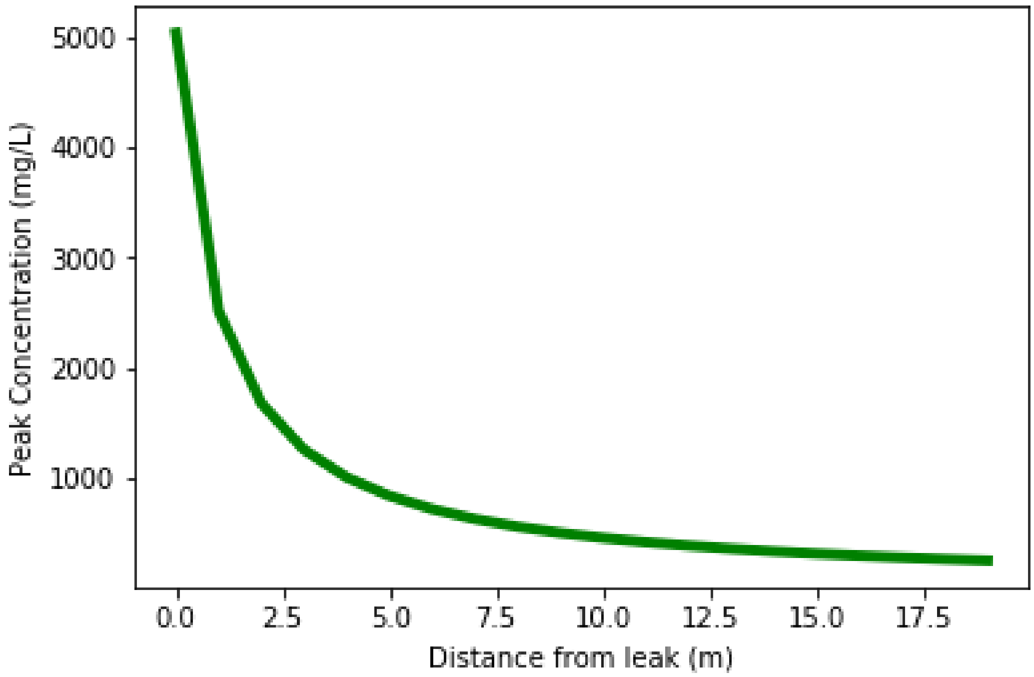
```
In [5]: # STEP 9: write output file
        f_out = open('pulse2D_output.txt','w')
        #f_out.write('t\tCmax\tsigma3x\tsigma3y\n')
        f_out.write('{:12}'.format('t')+'\t' \
                    +'{:12}'.format('Cmax')+'\t' \
                    +'{:12}'.format('sigma3x')+'\t' \
                    +'{:12}'.format('sigma3y')+'\n')
        for i in range(len(domain)):
            # convert all numbers to floats with 14 sig fig
            t = '{:04.10f}'.format(t_out[i])
            Cmax = '{:04.10f}'.format(Cmax_out[i])
            sigma3x = '{:04.10f}'.format(sigma3x_out[i])
            sigma3y = '{:04.10f}'.format(sigma3y_out[i])

            # convert to string for writing, format string width to 12 characters so that cols a
            t = '{:.12}'.format(str(t))
            Cmax = '{:.12}'.format(str(Cmax))
            sigma3x = '{:.12}'.format(str(sigma3x))
            sigma3y = '{:.12}'.format(str(sigma3y))
            strng = t + '\t' + Cmax + '\t' + sigma3x + '\t' + sigma3y + '\n'
            f_out.write(strng)

        f_out.close()
```

```
In [6]: # STEP 8: Plot data
        plt.figure(1)
        plt.plot(t_out,'r', linewidth=4)
        plt.xlabel('Distance from leak (m)')
        plt.ylabel('Plume travel time (days)')
        plt.show()

        plt.figure(2)
        plt.plot(Cmax_out,'g', linewidth=4)
        plt.xlabel('Distance from leak (m)')
        plt.ylabel('Peak Concentration (mg/L)')
        plt.show()

        plt.figure(3)
        plt.plot(sigma3x_out,'b', linewidth=4)
        plt.xlabel('Distance from leak (m)')
```

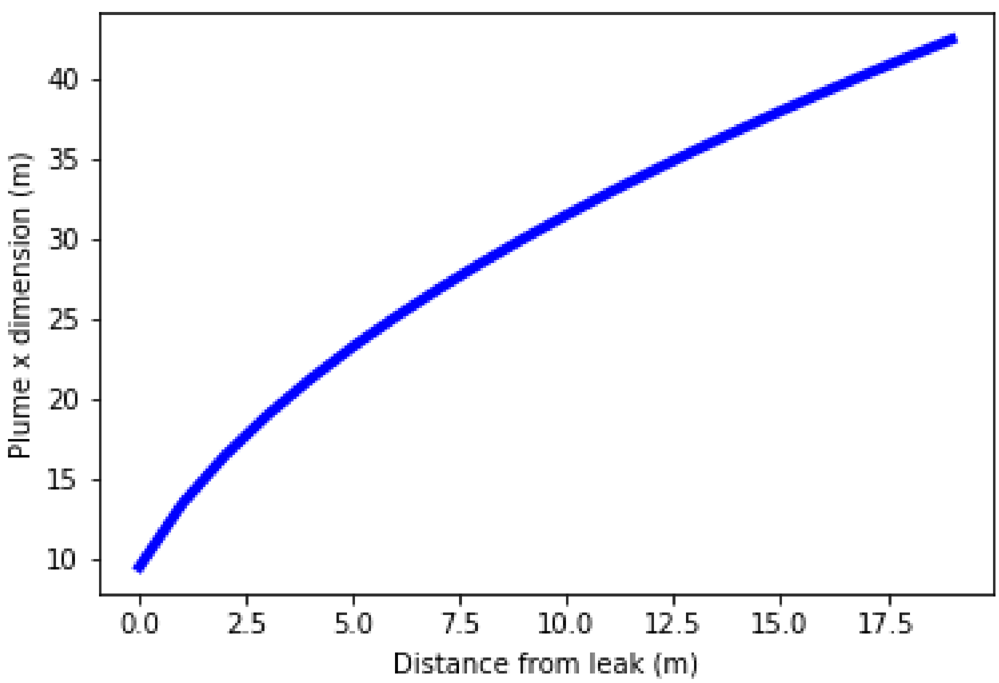
```
plt.ylabel('Plume x dimension (m)')
plt.show()

plt.figure(4)
plt.plot(sigma3y_out,'c', linewidth=4)
plt.xlabel('Distance from leak (m)')
plt.ylabel('Plume y dimension (m)')
plt.show()
```

```
C:\Users\kathe\Anaconda3\lib\site-packages\matplotlib\font_manager.py:1238: UserWarning: findfon
  (prop.get_family(), self.defaultFamily[fontext]))
```

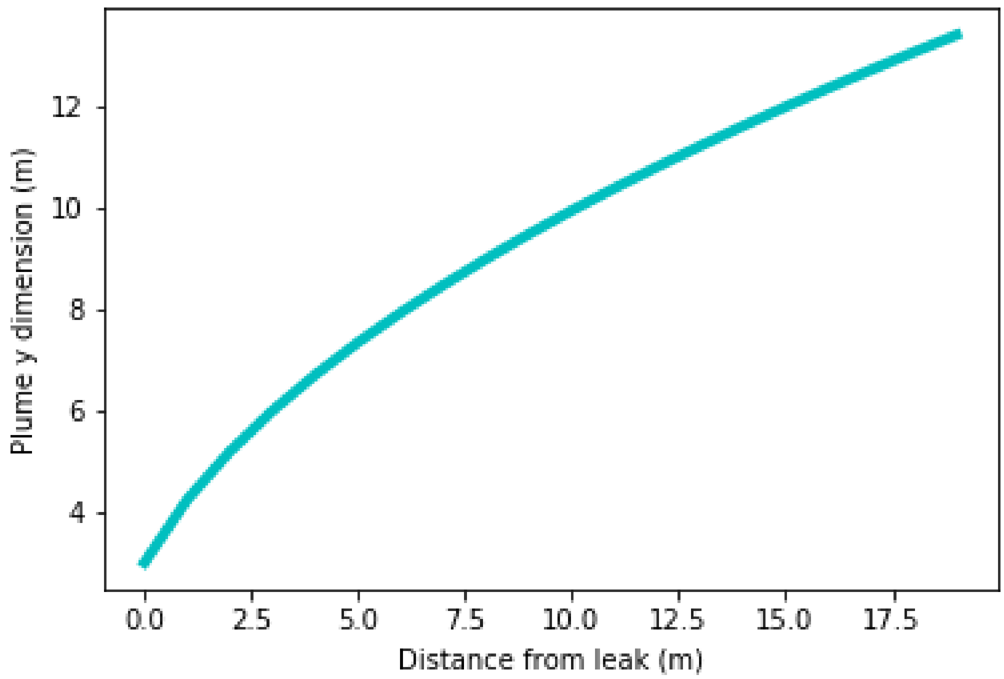




5000
4000
3000
2000
1000
Peak Concentration (mg/L)
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
Distance from leak (m)



40
35
30
25
20
15
10
Plume x dimension (m)
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
Distance from leak (m)



12
10
8
6
4
Plume y dimension (m)
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
Distance from leak (m)


```
In [ ]:
```