Time-variable inlet concentrations

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Overview

Demonstration of time-variable inlet gas concentrations of target compound.

R prep

Some R stuff.

```
library(reticulate)
```

```
# Find python executable
system('where python')
```

```
## Warning in system("where python"): error in running command
```

```
if(.Platform$OS.type == "windows") {
  use_python('C:\\Users\\sasha\\AppData\\Local\\Programs\\Python\\Python311')
} else {
  use_python('/usr/bin/python3')
}
```

And now the Python model

Import necessary packages

```
import shutil
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
```

Import model

```
shutil.copy('../../mod_funcs.py', '.')
```

```
## './mod_funcs.py'
```

```
from mod_funcs import tfmod
```

Set model inputs. See the notes in `tfmod.py` for more complete descriptions of inputs (and units).

```
L = 2           # Filter length/depth (m)
por_g = 0.5     # (m3/m3)
por_l = 0.25    # (m3/m3)
v_g = 0.03
v_l = 2E-5
```

```
nc = 30          # Number of model cells (layers)
cg0 = 1          # (g/m3)
cl0 = 0          # (g/m3)
henry = (0.1, 2000.)
temp = 15.       # (degrees C)
dens_l = 1000    # Liquid density (kg/m3)

k = 500. / 3600  # Reaction rate (1/s)

pH = 7.
pKa = 7.

# Time-variable dirty air concentration coming in
#                              ~~~~~~~Time in seconds~~~~~~~~~~~~~~           Concentration in g/m3
cgin = pd.DataFrame({'time': [0, 1000, 1100, 3600, 3700, 5000, 7200], 'cgin': [1, 3, 1, 1, 4, 2, 2]})
cgin = np.array([[0, 1000, 1100, 3600, 3700, 5000, 7200], [1, 3, 1, 1, 4, 2, 2]])
print(type(cgin))
```

```
## <class 'numpy.ndarray'>
```

```
print(type(cgin) is pd.core.frame.DataFrame)

# Fixed for water
```

```
## False
```

```
clin = 0.        # Fresh water concentration (g/m3)

# Times for model output, calculated from tt (total time) and nt (number of output times) here but coul
# Total duration (hours)
tt = 2
# Number of time rows
nt = 500
times = np.linspace(0, tt, nt) * 3600
```

Model scenarios

```
# Red line
Kga = 0.06
print(pred1)
```

```
## (array([[1.        , 0.92772896, 0.95589272, ..., 1.81175847, 1.81175847,
##          1.81175847],
##         [1.        , 0.83625418, 0.86398037, ..., 1.64155683, 1.64155683,
##          1.64155683],
##         [1.        , 0.75345132, 0.78085499, ..., 1.48734656, 1.48734656,
##          1.48734656],
##         ...,
##         [1.        , 0.24987754, 0.09060886, ..., 0.12627534, 0.12627534,
##          0.12627534],
##         [1.        , 0.2498745 , 0.08821567, ..., 0.11441285, 0.11441285,
##          0.11441285],
##         [1.        , 0.24987334, 0.08639314, ..., 0.10366474, 0.10366474,
##          0.10366474]]), array([[0.        , 1.13425774, 1.25534397, ..., 2.41871252, 2.41871252,
##          2.41871252],
##         [0.        , 1.02898238, 1.14208837, ..., 2.20763694, 2.20763694,
```

```
##          2.20763694],
##         [0.        , 0.9307638 , 1.03183682, ..., 2.00035601, 2.00035601,
##          2.00035601],
##         ...,
##         [0.        , 0.48489933, 0.18964364, ..., 0.16982978, 0.16982978,
##          0.16982978],
##         [0.        , 0.48489881, 0.18819167, ..., 0.15387573, 0.15387573,
##          0.15387573],
##         [0.        , 0.48489858, 0.18714667, ..., 0.13942041, 0.13942041,
##          0.13942041]]), array([[0.03333333, 0.0309243 , 0.03186309, ..., 0.06039195, 0.06039195,
##          0.06039195],
##         [0.03333333, 0.02787514, 0.02879935, ..., 0.05471856, 0.05471856,
##          0.05471856],
##         [0.03333333, 0.02511504, 0.0260285 , ..., 0.04957822, 0.04957822,
##          0.04957822],
##         ...,
##         [0.03333333, 0.00832925, 0.0030203 , ..., 0.00420918, 0.00420918,
##          0.00420918],
##         [0.03333333, 0.00832915, 0.00294052, ..., 0.00381376, 0.00381376,
##          0.00381376],
##         [0.03333333, 0.00832911, 0.00287977, ..., 0.00345549, 0.00345549,
##          0.00345549]]), array([[0.        , 0.0189043 , 0.0209224 , ..., 0.04031188, 0.04031188,
##          0.04031188],
##         [0.        , 0.01714971, 0.01903481, ..., 0.03679395, 0.03679395,
##          0.03679395],
##         [0.        , 0.01551273, 0.01719728, ..., 0.03333927, 0.03333927,
##          0.03333927],
##         ...,
##         [0.        , 0.00808166, 0.00316073, ..., 0.0028305 , 0.0028305 ,
##          0.0028305 ],
##         [0.        , 0.00808165, 0.00313653, ..., 0.0025646 , 0.0025646 ,
##          0.0025646 ],
##         [0.        , 0.00808164, 0.00311911, ..., 0.00232367, 0.00232367,
##          0.00232367]]), array([0.03333333, 0.1       , 0.16666667, 0.23333333, 0.3       ,
##        0.36666667, 0.43333333, 0.5       , 0.56666667, 0.63333333,
##        0.7       , 0.76666667, 0.83333333, 0.9       , 0.96666667,
##        1.03333333, 1.1       , 1.16666667, 1.23333333, 1.3       ,
##        1.36666667, 1.43333333, 1.5       , 1.56666667, 1.63333333,
##        1.7       , 1.76666667, 1.83333333, 1.9       , 1.96666667]), array([   0.        ,   14.42885
##          57.71543086,   72.14428858,   86.57314629,  101.00200401,
##         115.43086172,  129.85971944,  144.28857715,  158.71743487,
##         173.14629259,  187.5751503 ,  202.00400802,  216.43286573,
##         230.86172345,  245.29058116,  259.71943888,  274.14829659,
##         288.57715431,  303.00601202,  317.43486974,  331.86372745,
##         346.29258517,  360.72144289,  375.1503006 ,  389.57915832,
##         404.00801603,  418.43687375,  432.86573146,  447.29458918,
##         461.72344689,  476.15230461,  490.58116232,  505.01002004,
##         519.43887776,  533.86773547,  548.29659319,  562.7254509 ,
##         577.15430862,  591.58316633,  606.01202405,  620.44088176,
##         634.86973948,  649.29859719,  663.72745491,  678.15631263,
##         692.58517034,  707.01402806,  721.44288577,  735.87174349,
##         750.3006012 ,  764.72945892,  779.15831663,  793.58717435,
##         808.01603206,  822.44488978,  836.87374749,  851.30260521,
##         865.73146293,  880.16032064,  894.58917836,  909.01803607,
```

```
##         923.44689379,  937.8757515 ,  952.30460922,  966.73346693,
##         981.16232465,  995.59118236, 1010.02004008, 1024.4488978 ,
##        1038.87775551, 1053.30661323, 1067.73547094, 1082.16432866,
##        1096.59318637, 1111.02204409, 1125.4509018 , 1139.87975952,
##        1154.30861723, 1168.73747495, 1183.16633267, 1197.59519038,
##        1212.0240481 , 1226.45290581, 1240.88176353, 1255.31062124,
##        1269.73947896, 1284.16833667, 1298.59719439, 1313.0260521 ,
##        1327.45490982, 1341.88376754, 1356.31262525, 1370.74148297,
##        1385.17034068, 1399.5991984 , 1414.02805611, 1428.45691383,
##        1442.88577154, 1457.31462926, 1471.74348697, 1486.17234469,
##        1500.6012024 , 1515.03006012, 1529.45891784, 1543.88777555,
##        1558.31663327, 1572.74549098, 1587.1743487 , 1601.60320641,
##        1616.03206413, 1630.46092184, 1644.88977956, 1659.31863727,
##        1673.74749499, 1688.17635271, 1702.60521042, 1717.03406814,
##        1731.46292585, 1745.89178357, 1760.32064128, 1774.749499  ,
##        1789.17835671, 1803.60721443, 1818.03607214, 1832.46492986,
##        1846.89378758, 1861.32264529, 1875.75150301, 1890.18036072,
##        1904.60921844, 1919.03807615, 1933.46693387, 1947.89579158,
##        1962.3246493 , 1976.75350701, 1991.18236473, 2005.61122244,
##        2020.04008016, 2034.46893788, 2048.89779559, 2063.32665331,
##        2077.75551102, 2092.18436874, 2106.61322645, 2121.04208417,
##        2135.47094188, 2149.8997996 , 2164.32865731, 2178.75751503,
##        2193.18637275, 2207.61523046, 2222.04408818, 2236.47294589,
##        2250.90180361, 2265.33066132, 2279.75951904, 2294.18837675,
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##        2654.90981964, 2669.33867735, 2683.76753507, 2698.19639279,
##        2712.6252505 , 2727.05410822, 2741.48296593, 2755.91182365,
##        2770.34068136, 2784.76953908, 2799.19839679, 2813.62725451,
##        2828.05611222, 2842.48496994, 2856.91382766, 2871.34268537,
##        2885.77154309, 2900.2004008 , 2914.62925852, 2929.05811623,
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##        3001.20240481, 3015.63126253, 3030.06012024, 3044.48897796,
##        3058.91783567, 3073.34669339, 3087.7755511 , 3102.20440882,
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##        3174.34869739, 3188.77755511, 3203.20641283, 3217.63527054,
##        3232.06412826, 3246.49298597, 3260.92184369, 3275.3507014 ,
##        3289.77955912, 3304.20841683, 3318.63727455, 3333.06613226,
##        3347.49498998, 3361.9238477 , 3376.35270541, 3390.78156313,
##        3405.21042084, 3419.63927856, 3434.06813627, 3448.49699399,
##        3462.9258517 , 3477.35470942, 3491.78356713, 3506.21242485,
##        3520.64128257, 3535.07014028, 3549.498998  , 3563.92785571,
##        3578.35671343, 3592.78557114, 3607.21442886, 3621.64328657,
##        3636.07214429, 3650.501002  , 3664.92985972, 3679.35871743,
##        3693.78757515, 3708.21643287, 3722.64529058, 3737.0741483 ,
##        3751.50300601, 3765.93186373, 3780.36072144, 3794.78957916,
##        3809.21843687, 3823.64729459, 3838.0761523 , 3852.50501002,
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##        3924.6492986 , 3939.07815631, 3953.50701403, 3967.93587174,
##        3982.36472946, 3996.79358717, 4011.22244489, 4025.65130261,
```

```
##        4040.08016032, 4054.50901804, 4068.93787575, 4083.36673347,
##        4097.79559118, 4112.2244489 , 4126.65330661, 4141.08216433,
##        4155.51102204, 4169.93987976, 4184.36873747, 4198.79759519,
##        4213.22645291, 4227.65531062, 4242.08416834, 4256.51302605,
##        4270.94188377, 4285.37074148, 4299.7995992 , 4314.22845691,
##        4328.65731463, 4343.08617234, 4357.51503006, 4371.94388778,
##        4386.37274549, 4400.80160321, 4415.23046092, 4429.65931864,
##        4444.08817635, 4458.51703407, 4472.94589178, 4487.3747495 ,
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##        4905.81162325, 4920.24048096, 4934.66933868, 4949.09819639,
##        4963.52705411, 4977.95591182, 4992.38476954, 5006.81362725,
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##        5078.95791583, 5093.38677355, 5107.81563126, 5122.24448898,
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##        5194.38877756, 5208.81763527, 5223.24649299, 5237.6753507 ,
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##        5367.53507014, 5381.96392786, 5396.39278557, 5410.82164329,
##        5425.250501  , 5439.67935872, 5454.10821643, 5468.53707415,
##        5482.96593186, 5497.39478958, 5511.82364729, 5526.25250501,
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##        6175.5511022 , 6189.97995992, 6204.40881764, 6218.83767535,
##        6233.26653307, 6247.69539078, 6262.1242485 , 6276.55310621,
##        6290.98196393, 6305.41082164, 6319.83967936, 6334.26853707,
##        6348.69739479, 6363.12625251, 6377.55511022, 6391.98396794,
##        6406.41282565, 6420.84168337, 6435.27054108, 6449.6993988 ,
##        6464.12825651, 6478.55711423, 6492.98597194, 6507.41482966,
##        6521.84368737, 6536.27254509, 6550.70140281, 6565.13026052,
##        6579.55911824, 6593.98797595, 6608.41683367, 6622.84569138,
##        6637.2745491 , 6651.70340681, 6666.13226453, 6680.56112224,
##        6694.98997996, 6709.41883768, 6723.84769539, 6738.27655311,
##        6752.70541082, 6767.13426854, 6781.56312625, 6795.99198397,
##        6810.42084168, 6824.8496994 , 6839.27855711, 6853.70741483,
##        6868.13627255, 6882.56513026, 6896.99398798, 6911.42284569,
##        6925.85170341, 6940.28056112, 6954.70941884, 6969.13827655,
##        6983.56713427, 6997.99599198, 7012.4248497 , 7026.85370741,
##        7041.28256513, 7055.71142285, 7070.14028056, 7084.56913828,
##        7098.99799599, 7113.42685371, 7127.85571142, 7142.28456914,
```

```
##       7156.71342685, 7171.14228457, 7185.57114228, 7200.       ]), 33.333333333333336, 24999.99999
```

```
pred1 = tfmod(L = L, por_g = por_g, por_l = por_l, v_g = v_g, v_l = v_l, nc = nc, cg0 = cg0,
              cl0 = cl0, cgin = cgin, clin = clin, Kga = Kga, k = k, henry = henry, pKa = pKa,
              pH = pH, temp = temp, dens_l = dens_l, times = times)

# Onda correlation
# Blue line in plots
pred2 = tfmod(L = L, por_g = por_g, por_l = por_l, v_g = v_g, v_l = v_l, nc = nc, cg0 = cg0,
              cl0 = cl0, cgin = cgin, clin = clin, Kga = 'onda', k = k, henry = henry, pKa = pKa,
              pH = pH, temp = temp, dens_l = dens_l, times = times)

# Turn off reaction to see concentration change
# Green line in plots
k = 0.
pred3 = tfmod(L = L, por_g = por_g, por_l = por_l,v_g = v_g, v_l = v_l, nc = nc, cg0 = cg0,
              cl0 = cl0, cgin = cgin, clin = clin, Kga = 'onda', k = k, henry = henry, pKa = pKa,
              pH = pH, temp = temp, dens_l = dens_l, times = times)
```

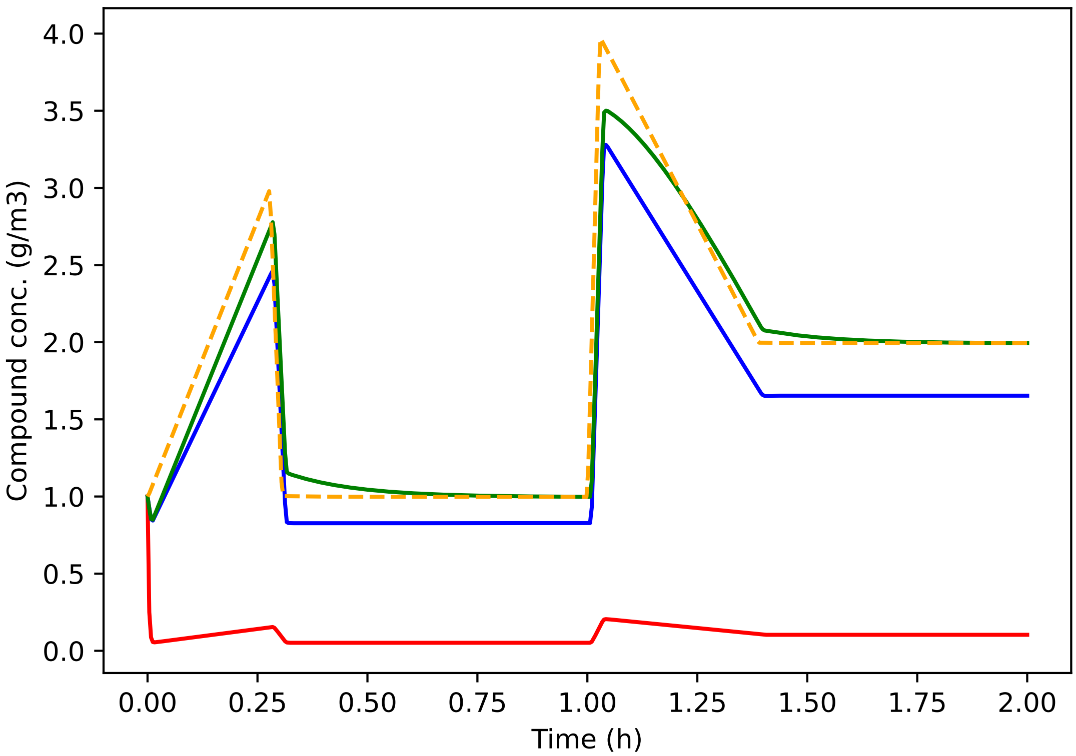
Check Kga

```
pred2[8]
```

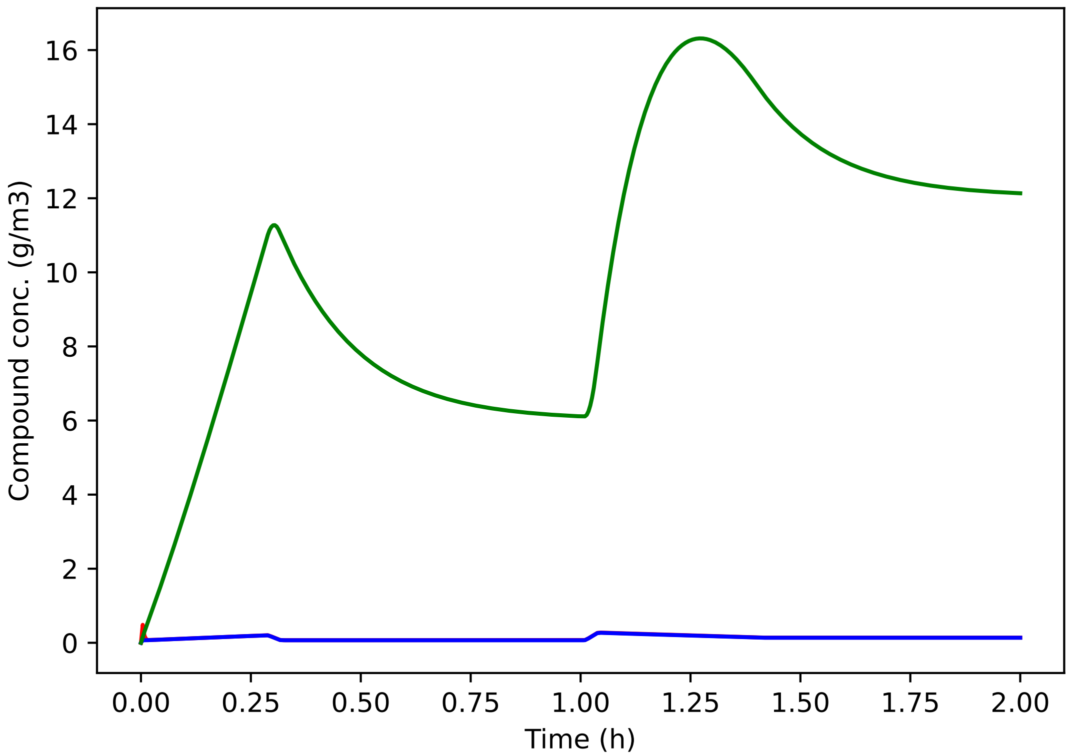
```
## 0.0029026318924857734
```

Plots

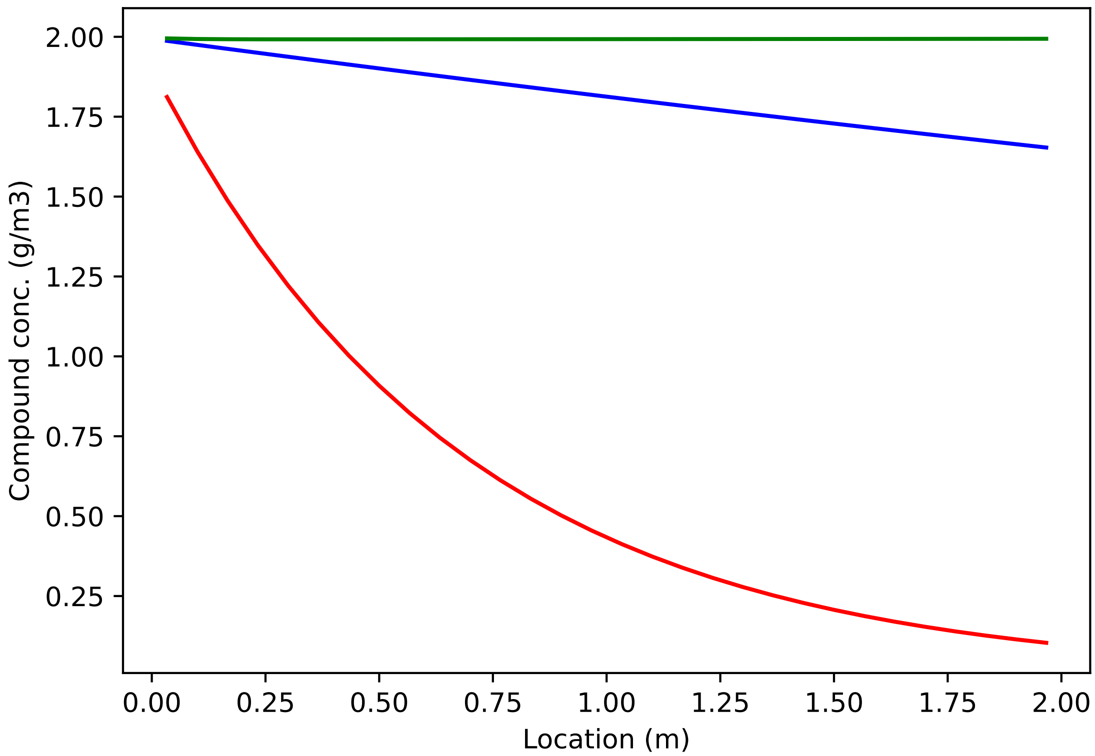
```
# Plot outlet concentration (= 1 - removal efficiency here because cgin = 1)
# Gas concentration (outlet air)
plt.plot(pred1[5] / 3600, pred1[0][nc - 1, :], 'r-')
plt.plot(pred2[5] / 3600, pred2[0][nc - 1, :], 'b')
plt.plot(pred3[5] / 3600, pred3[0][nc - 1, :], 'g-')
plt.plot(pred3[5] / 3600, pred3[0][0, :], 'orange', linestyle = 'dashed')
plt.xlabel('Time (h)')
plt.ylabel('Compound conc. (g/m3)')
```



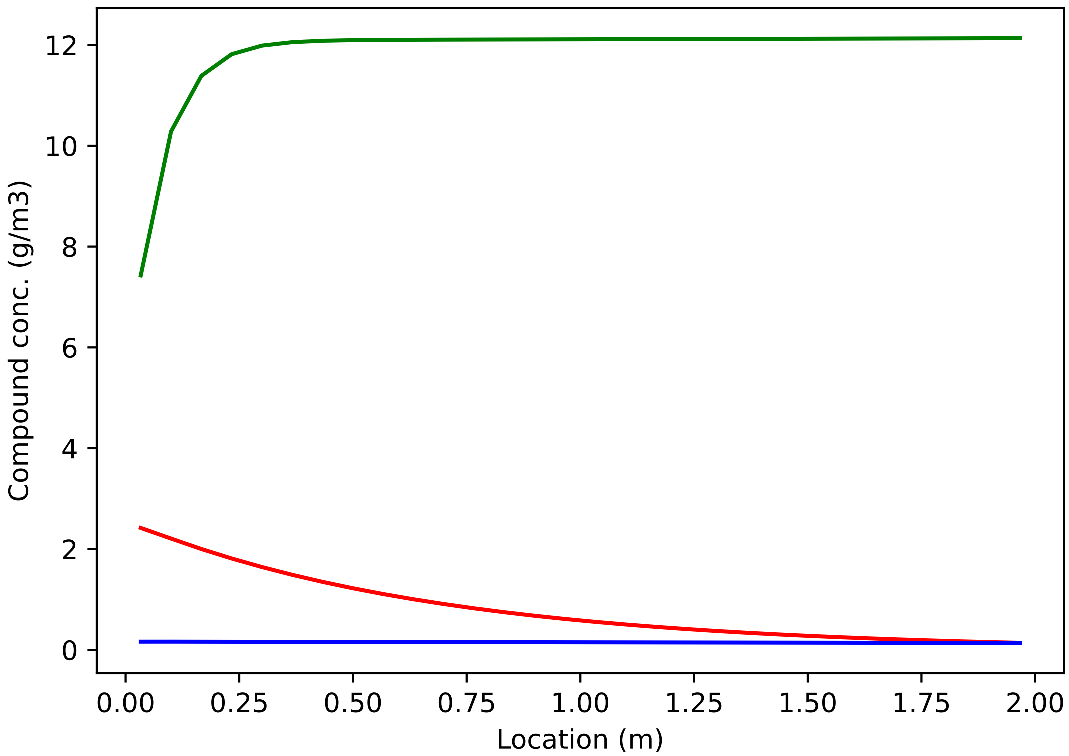

```
# Liquid concentration (in last layer)
plt.clf()
plt.plot(pred1[5] / 3600, pred1[1][nc - 1, :], 'r-')
plt.plot(pred2[5] / 3600, pred2[1][nc - 1, :], 'b')
plt.plot(pred3[5] / 3600, pred3[1][nc - 1, :], 'g-')
plt.xlabel('Time (h)')
plt.ylabel('Compound conc. (g/m3)')
```




```
# Profiles
# Gas
plt.clf()
plt.plot(pred1[4], pred1[0][:, nt - 1], 'r-')
plt.plot(pred2[4], pred2[0][:, nt - 1], 'b')
plt.plot(pred3[4], pred3[0][:, nt - 1], 'g-')
plt.xlabel('Location (m)')
plt.ylabel('Compound conc. (g/m3)')
```




```
# Liquid
plt.clf()
plt.plot(pred1[4], pred1[1][:, nt - 1], 'r-')
plt.plot(pred2[4], pred2[1][:, nt - 1], 'b')
plt.plot(pred3[4], pred3[1][:, nt - 1], 'g-')
plt.xlabel('Location (m)')
plt.ylabel('Compound conc. (g/m3)')
```



Compound conc. (g/m3)
12
10
8
6
4
2
0
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00
Location (m)