Time-variable inlet concentrations

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Overview

Demonstration of time-variable inlet gas concentrations of target compound. This is done in R Markdown because there is no simple equivalent for Python and the reticulate package lets R do Python stuff.

This file should work on Windows or Linux (although the location of the python executable will have to be manually set, annoyingly).

Steps on Windows

First time

1. Install reticulate package in R
2. Open this Rmd file in RStudio
3. Set working directory to "source file location" (Session -> Set working dir -> Source file location)
4. Set Python executable location in block below if it is not correct (Anders, you can change it permanently to your path below)
5. "Knit" document

After that

1. Open this Rmd file in RStudio
2. Set working directory to "source file location" (Session -> Set working dir -> Source file location)
3. "Knit" document

R prep

Some R stuff.

```
library(reticulate)
```

```
## Warning: package 'reticulate' was built under R version 4.1.3
```

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

```
## [1] 0
```

```
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 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 = np.array([[0, 1000, 1100, 3600, 3700, 5000, 7200], [1, 3, 1, 1, 4, 2, 2]])
# Fixed for water
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
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)
```

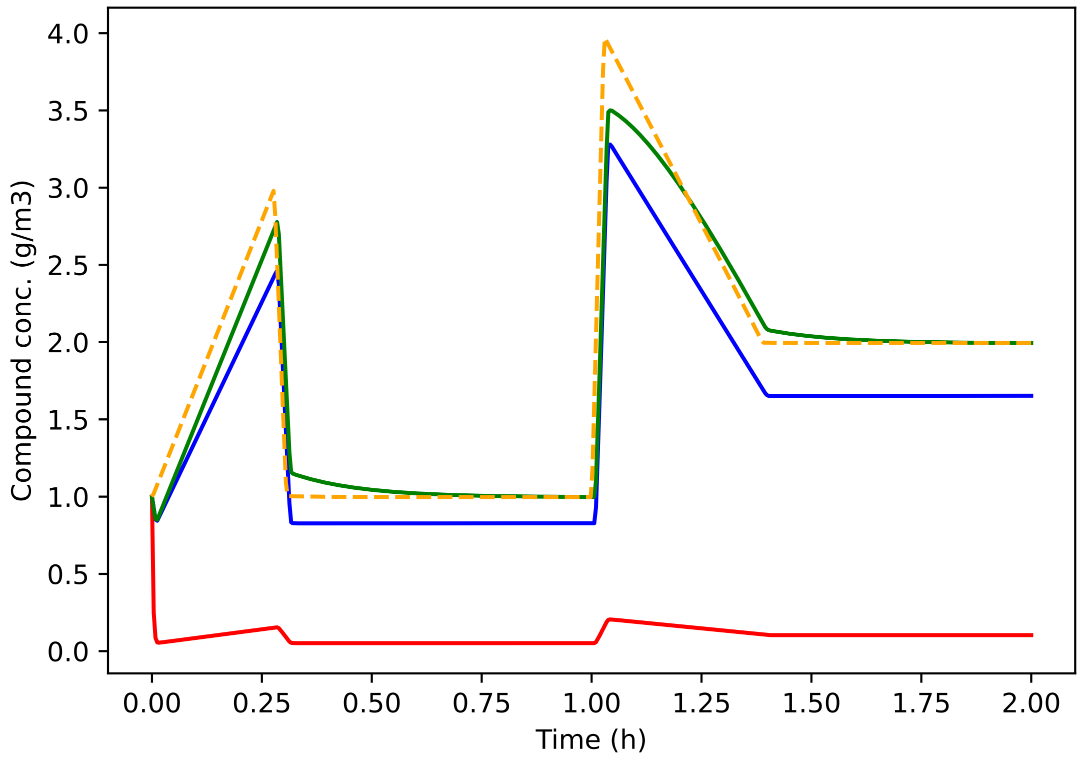
Check Kga

```
pred2[8]
```

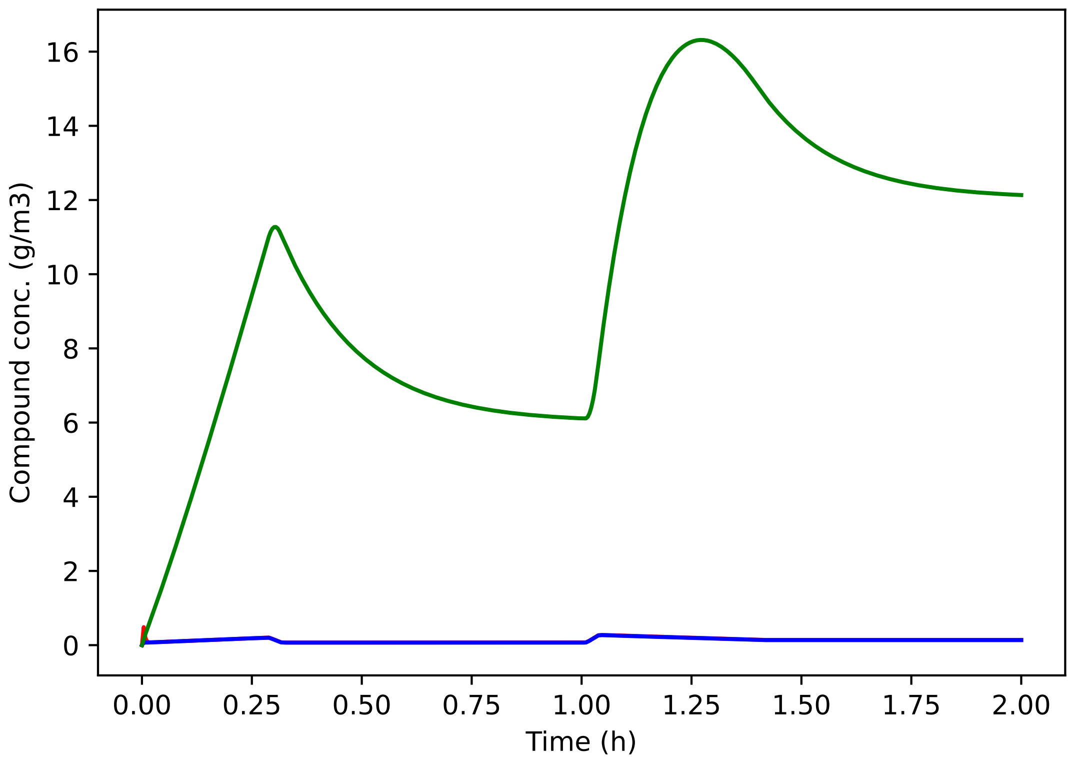
```
## 0.0029026318924857734
```

Plots

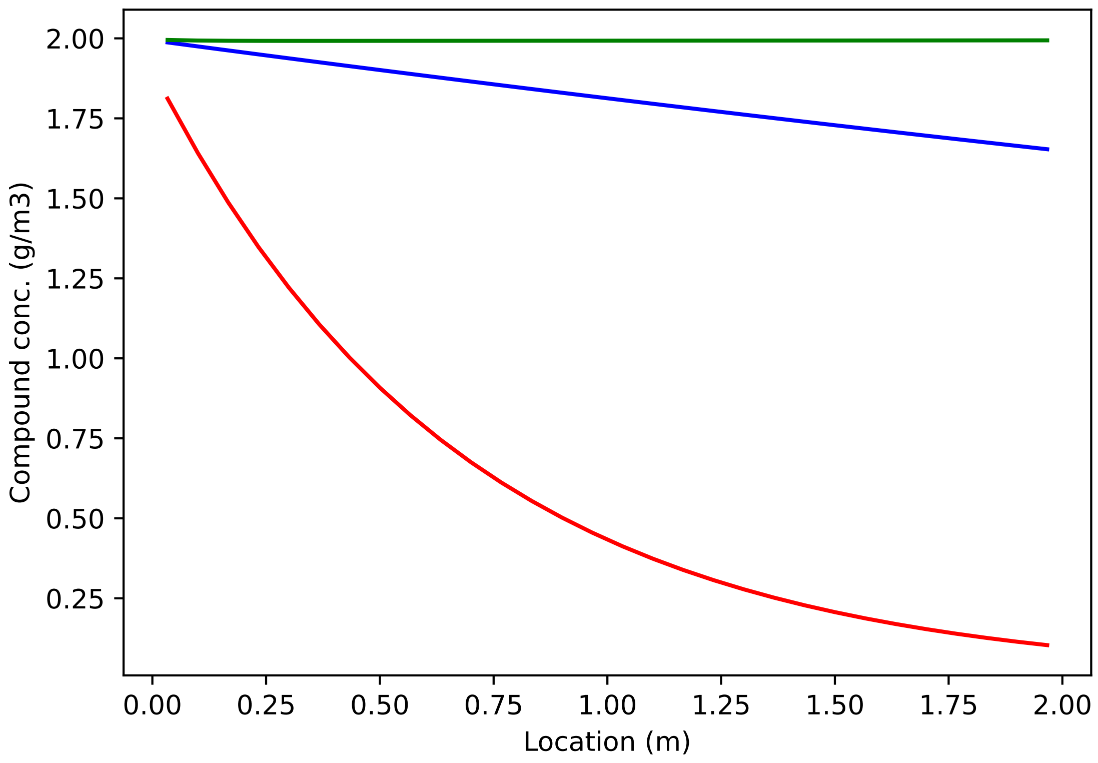
```
# Plot outlet concentration (= 1 - removal efficiency here because cgin = 1)
# Gas concentration (outlet air)
plt.plot(pred1[5] / 3600, pred1[0][nc - 1, :], 'r-')
plt.plot(pred2[5] / 3600, pred2[0][nc - 1, :], 'b')
plt.plot(pred3[5] / 3600, pred3[0][nc - 1, :], 'g-')
plt.plot(pred3[5] / 3600, pred3[0][0,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



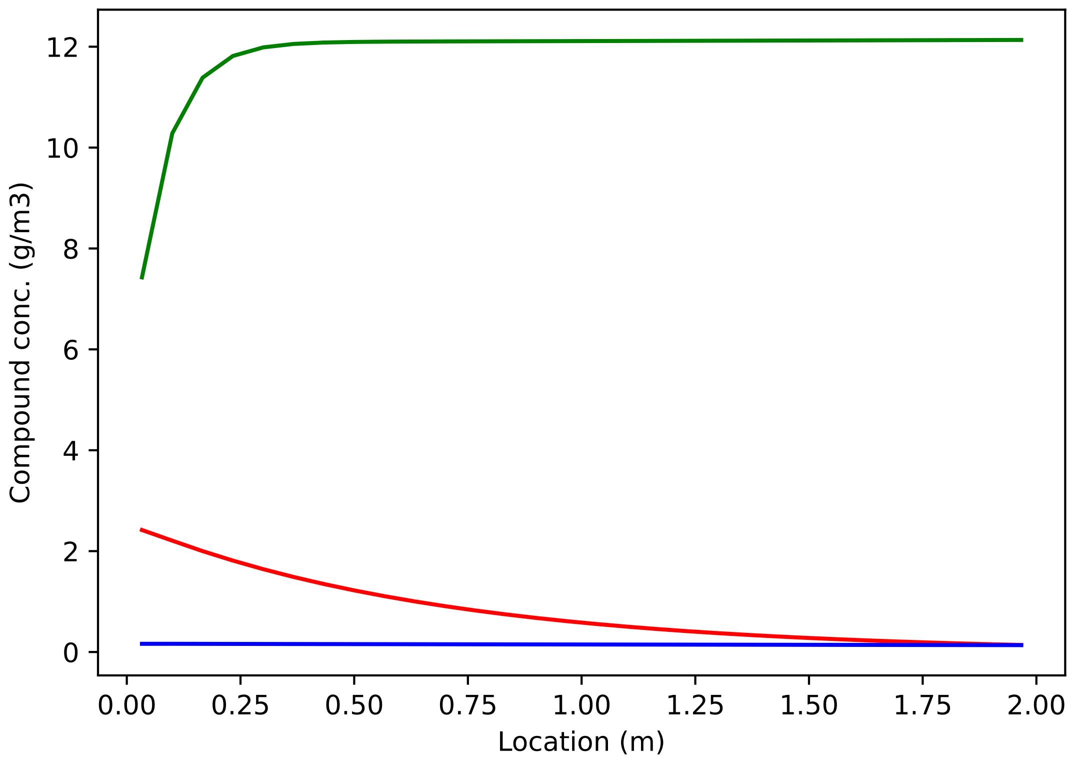
```python
# Liquid concentration (in last layer)
plt.clf()
plt.plot(pred1[5] / 3600, pred1[1][nc - 1, :], 'r-')
plt.plot(pred2[5] / 3600, pred2[1][nc - 1, :], 'b')
plt.plot(pred3[5] / 3600, pred3[1][nc - 1, :], 'g-')
plt.xlabel('Time (h)')
plt.ylabel('Compound conc. (g/m3)')
```



```python
# 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)