ch4_transport_example

May 29, 2023

1 Gas transport model for CH4 transport in a tree

This notebook shows how the gas transport model localted in folder transport_model can be run to solve CH4 transport in a tree. The input parameters used here are not complitely realistic but hopefully demonstrates what the model needs in order to run.

2 How to run this notebook

This notebook is written using Jupyter notebooks and Python (version 3.9.16 but also newer versions should work). You can go through the notebook and look at the figures produced from the gas transport model output without doing anything by simply opening the .html version of the notebook on your browser. If you would like to run the notebook and edit input parameters you need to:

- 1. Install python (at least version 3.9.16) from getpython.org and pip. You can follow for example these instructions on windows linuxhint. For other operating systems you can search instructions for example with "install python and pip [your operating system]" and "create python virtual environment [your operating system]"
- 2. Create a virtual environment using terminal or command prompt

>> python -m venv ch4venv

- You can read more about virtual environments and what they are from here
- 3. Activate the virtual environment using terminal or command prompt

>> source ch4venv/bin/activate

4. Install the required python packages using terminal or command prompt

(ch4venv) >> pip install -r requirements.txt

5. Start jupyter notebook server using terminal or command prompt

(ch4venv) >> jupyter-notebook

- A web browser should open which should show the contents of this directory. Click the file "ch4_transport_example.ipynb"
 - If a browser window does not open copy the link given in the terminal and navigate to it using your browser
- You can run cells by clicking "Run cell" from the top toolbar or by pressing "ctrl + enter"

- 6. (optional) You can modify input values and then run the model again. To run the model again with your modifications
 - Either remove file "ch4_transport_test_out.nc" or rename the variable called 'output-file'
 - Run the whole notebook again from top menu Cell->Run all

```
[]: import numpy as np
import xarray as xr

import matplotlib.pyplot as plt
import seaborn as sns

from transport_model.gas import Gas

sns.set_context('notebook')

%load_ext autoreload
%autoreload 2
```

The autoreload extension is already loaded. To reload it, use: %reload_ext autoreload

3 Model input

3.1 Table of all the model input and output parameters

These parameters are set below

Input parameter	Unit	Notes
Tree height	m	
Tree radius	m	
Axial resolution	m	Can be tested to find a good value
Radial resolution	m	Can be tested to find a good value
Simulation time	S	
Henry's law coefficient for CH4	m3 air / m3 water	From the literature
Initial CH4 concentration	mol/m3	Can be approximated and run the model for a "burn in" period to allow the system to reach equilibrium
Sapflow velocity	m/s	
Xylem to heartwood ratio	-	by area or by length
Radial diffusion coefficient of CH4 in the tree	m2/s	
Axial diffusion coefficient of CH4 in the tree	m2/s	

Input parameter	Unit	Notes
equilibration rate between gas and aqueous phase CH4	1/s	Can be set to high value for instantenous equilibrium?
Volume fraction of air in the tree	_	•
Volume fraction of water in the tree	_	
Volume fraction of cell in the tree	-	
Uptake rate of water from the roots	m3/s	If CH4 transport from soil through root water uptake is modelled
CH4 concentration in the soil	m mol/m3	If CH4 transport from soil
		through root water uptake is modelled
Strengths of other source and sink processes	mol/s	If other sources are modelled
Ambient gas phase concentration of CH4	mol/m3	Also in the soil
Name of the output file	-	
Max lines per time step		Currently, this is suggested to be set as 1 and control the time step manually e.g., in this notebook we set the time step to one hour but could use 5 mins as well. The model has it's own intrinsic (dynamic) time step which it uses to run the model manually specified time step at a time

3.2 Tree dimensions

First we need to define how many axial and radial elements the model has and what is the length and height of each element.

We'll model a tree whose height is $10~\mathrm{m}$ and radius $5~\mathrm{cm}$ and whose roots reach depth of $0.5~\mathrm{meters}$. The model will have $105~\mathrm{axial}$ elements and $10~\mathrm{radial}$ elements corresponding to axial resolution of $10~\mathrm{cm}$ and radial resolution of $0.5~\mathrm{cm}$

```
element_radius = np.repeat([tree_radius/nr], repeats=na*nr).reshape(na,nr)
```

3.3 Simulation time

Next we need to set the simulation time. We'll simulate the transport of CH4 for two weeks with 1 hour time interval. The 1h time interval will be used to update the sapflow velocity and root water uptake rates.

```
[]: simulation_time = np.linspace(0,14*24*60*60, 14*24+1) # simulation time in seconds
```

3.4 Initial CH4 concentration

Next, we need to define the amount of CH4 the tree has initially in both gas and aqueous phases. Here We'll assume that the tree is initially in equilibrium with atmospheric concentration of 1900 ppb

3.4.1 We'll first define the gas phase concentration

```
atmospheric_ch4_concentration_ppb = 1900 #(ppb; nmol ch4 / mol air)

atmospheric_pressure = 101325 # Atmospheric pressure (Pa)

temperature = 281 # (K)

R = 8.3145 # Molar gas constant (J/K/mol)

atmospheric_ch4_concentration_mol_m3 = atmospheric_ch4_concentration_ppb *_
→atmospheric_pressure / (temperature * R) * 1e-9# The model needs the_
→concentration in mol/m^3
```

```
[]: tree_ch4_gas_concentration = np.repeat([atmospheric_ch4_concentration_mol_m3],__
repeats=na*nr).reshape(na,nr)
```

3.4.2 Next we set the aqueous phase concentration using Henry's law

```
[]: kh = 1.4e-5*temperature*R # Henry's law coefficient at 298.15 [K] = m3 air / m3_\( \text{water}\)
tree_ch4_aqueos_concentration = tree_ch4_gas_concentration.copy()*kh
```

3.4.3 Combine the concentrations to one 3D array

The dimensions of the ch4_concentration array are (na,nr,2). In the last dimension first index is for gas phase concentration and second for the aqueous phase

3.5 Sapflow velocity

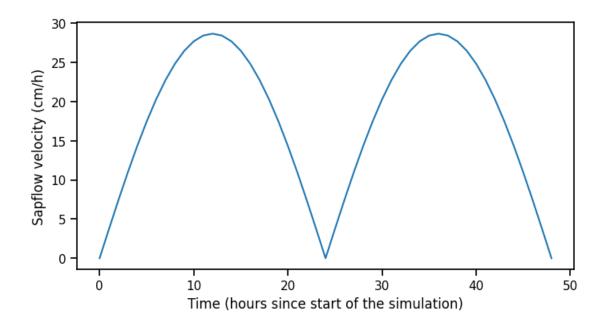
instead of sapflow density, the model input is sapflow velocity in units m/s. Here we'll assume that the sapflow density is the same throughout the tree and follows sine-wave with maximum at ~ 30 cm/h and that from the basal area of the tree 20% is heartwood and 80% xylem.

3.5.1 Define which elements belong to heartwood

The heartwood area should be 20% of the total area

3.5.2 Visualize sapflow velocity

```
[]: Text(0, 0.5, 'Sapflow velocity (cm/h)')
```



3.6 CH4 diffusion coefficients

Next we'll set radial and axial diffusion coefficients. We'll assume same value (1.5e-8 m2/s) for radial diffusion and set the axial diffusion coefficient to be same as diffusion coefficient of CH4 in air.

```
[]: D_ch4_gas_radial = np.repeat([1.5e-8], repeats=na*nr).reshape(na,nr) # m^2/s
D_ch4_gas_axial = np.repeat([2e-5], repeats=na*nr).reshape(na,nr) # m^2/s
```

3.7 Equilibration rate

The equilibration rate determines the rate at which gas and aquoues phases approach equilibrium given by the Henry's law. Here we set the equilibration rate to high value which leads to fast equilibration.

```
[]: eq_rate = 0.1 # 1/s
```

3.8 Space division

Next, we need to set volume fraction of air and aqueous phases and cell in the tree. We'll use same values for each element

```
[]: w_gas = np.repeat([0.2], na*nr).reshape(na,nr)
w_aq = np.repeat([0.4], na*nr).reshape(na,nr)

w_cell = np.repeat([0.4], na*nr).reshape(na,nr)

space_division = np.stack((w_gas, w_aq, w_cell), axis=2)
```

3.9 CH4 uptake through the roots

Next, we need to determine how much CH4 enters the model via root water uptake (RWU). For this we need to determine first the root water uptake rate in m3/s and then the soil aqueous phase CH4 concentration.

In this example we'll assume that the storage change in the tree is zero in every element i.e., that the RWU rate = Transpiration rate and further, that the transpiration rate equals sapflow density. We'll distribute the RWU rate at different soil depths using an exponential decay function. More precise determination would require calculating RWU explicitly which in turn requires knowledge how roots of the tree are distributed and how much roots the tree has in total.

For soil aqueous phase CH4 concentration we set a total value of 1 mmol/m3 (=1 \$ \$ mol/l) and similar to RWU assume that the concentration decreases exponentially as a function of soil depth.

3.9.1 Root water uptake rate

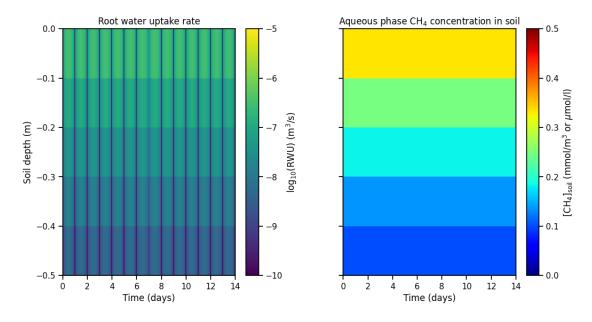
```
[]: # Initialize RWU and soil aqueous phase CH4 concentration arrays.
     # The model needs the length of both of these arrays to be the same as the
      ⇔number of axial elements
     # but there should be only zeros in elements which are above ground
     RWU = np.zeros((na,simulation_time.shape[0]-1)) # Root water uptake rate (m^3/s)
     # Define soil depth at the end and middle of each root element (total 5_{\sqcup}
      elements since rooting depth was set to 0.5 m and axial resolution is 10 cm)
     z soil = np.cumsum(element_heights[-5:,0]) # soil layer depth at the end of the_
      \Rightarrow layer (m); z_soil = array([0.1, 0.2, 0.3, 0.4, 0.5])
     z_middle = np.insert(z_soil, 0, 0.0)
     z_middle[:-1] = z_middle[:-1] + np.diff(z_middle)/2.0
     z_{middle} = z_{middle}[:-1] # soil depth at middle of each layer (m) <math>z_{middle} = 0
      \hookrightarrow array([0.05, 0.15, 0.25, 0.35, 0.45])
     # Define total RWU to be distributed among the 5 root layers
     RWU_sum = sapflow_density[1:].reshape(sapflow_density.shape[0]-1, 1) # Total_
      \rightarrowrate of water taken up by the roots in a time step (m^3/s)
     RWU_scale = np.exp(-z_middle*10) # % how much of RWU_sum comes from different_
      \neg root\ layers\ RWU\ scale = array([0.60653066,\ 0.22313016,\ 0.082085\ ,\ 0.
      ⇔03019738, 0.011109 ])
     RWU_scale = RWU_scale/np.sum(RWU_scale) # Normalize to unity RWU_scale =_ 
      -array([0.63640865, 0.23412166, 0.08612854, 0.03168492, 0.01165623])
     RWU_scale = RWU_scale.reshape(RWU_scale.shape[0], 1) # reshape for matrix_
      \rightarrow multiplication
```

3.9.2 CH4 concentration in the soil

The difference between CH4 soil aq concentration array and the RWU array is that in this example we'll keep the soil CH4 concentration constant in time.

3.9.3 Visualize RWU and CH4 concentration in the soil

[]: Text(0.5, 1.0, 'Aqueous phase CH\$_4\$ concentration in soil')



3.10 Other sources and sinks

The model allows also definition of other CH4 sources and sinks. In this example we set one source at ~ 8 m height and one sink at ~ 0.1 m height. The source / sink strength is calculated from the current gas phase concentration for every time step

```
[]: # Define tree height at the middle of the tree. This is needed later.

tree_height_middle = np.cumsum(element_heights[:, 0])

tree_height_middle = np.insert(tree_height_middle, 0, 0.0)

tree_height_middle = tree_height_middle - 0.5 # substract the rooting depth

tree_height_middle[:-1] = tree_height_middle[:-1] + np.diff(tree_height_middle)/

$\times 2.0$

tree_height_middle = tree_height_middle[:-1]
```

```
tree_height_middle = np.flip(tree_height_middle) # This flip is required since_u 
in the model first index is at the top of the tree
```

```
[]: def source and sink(current molar amount):
         source_and_sink = np.zeros((na, nr, 2)) # the dimensions of the array need_
      →to be the same as the current molar amount array's. The each element of the
      ⇒source and sink array needs to be in units mol/s
         # define a source at ca. 8 m height
         ind_8m = np.argmin(np.abs(tree_height_middle-8))
         source_strength = 5e-11 # (mol/s)
         source and sink[ind 8m, :, 0] = source strength
         # define a sink at ca. 0.1 m height
         ind_01m = np.argmin(np.abs(tree_height_middle-0.1))
         sink_strength = 1e-4 # (1/s) need to be careful with this value since it_
      →applies for one hour before it is updated and can lead to negative
      \hookrightarrow concentrations
         source_and_sink[ind_01m, :, 0] = -1.0*current_molar_amount[ind_01m, :, 0] *_
      ⇔sink strength
         return source_and_sink
```

3.11 Concentration outside the stem

Next we need to set the atmospheric concentration and the concentration in the soil in gas phase. We'll use the value for atmospheric concentration and assume that the soil aqueous and gas phases are in equilibrium.

3.12 Output file and number of lines to save in a timestep

Lastly, we need to set the name of the output file and how many lines we want to save there in each time step. Currently the value of the fluxes can only be saved if number of outputlines per timestep is 1. The results are saved in a NetCDF file.

```
[]: outputfile = 'ch4_transport_test_out.nc'
    output_lines_per_step = 1
```

4 Initialize the model

```
[]: model = Gas(num_axial_elements=na,
                 num radial elements=nr,
                 element_height=element_heights,
                 element_length = element_radius,
                 radial_diffusion_coefficient=D_ch4_gas_radial,
                 axial_diffusion_coefficient=D_ch4_gas_axial,
                 equilibration rate=eq rate,
                 velocity=sapflow_velocity_whole_tree[:, :, 0],
                 space_division=space_division,
                 concentration=ch4_concentration,
                 henrys_law_coefficient=kh,
                 temperature=temperature,
                 ambient_concentration= ambient_concentration,
                 sources_and_sinks=np.zeros((na,nr,2)),
                 soil_compound_aq_concentration=ch4_soil_aq_concentration,
                 axial_water_uptake=RWU[:, 0].reshape(na,1),
                 outputfile=outputfile,
                 max_output_lines=output_lines_per_step
                 )
```

5 Run the model

Running the model takes 1-2 minutes

```
for i, t in enumerate(simulation_time[:-1]):
    if t%86400 == 0:
        print(f'Days elapsed: {t/86400}')
    # update sapflow velocity, source and sink strength and root water uptake_
    *rate
    model.velocity = sapflow_velocity_whole_tree[:, :, i]
    model.sources_and_sinks = source_and_sink(model.n_in)
    model.axial_water_uptake = RWU[:, i].reshape(na,1)

#run for one time step (one hour

model.run(time_start = t, time_end = simulation_time[i+1])

print('Simulation ready')
```

```
Days elapsed: 0.0
Days elapsed: 1.0
Days elapsed: 2.0
Days elapsed: 3.0
Days elapsed: 4.0
Days elapsed: 5.0
Days elapsed: 6.0
Days elapsed: 7.0
Days elapsed: 8.0
Days elapsed: 9.0
Days elapsed: 10.0
Days elapsed: 11.0
Days elapsed: 12.0
Days elapsed: 13.0
Simulation ready
```

5.0.1 Close the netcdf output file

```
[ ]: model.ncf.close()
```

6 Visualize model output

6.1 Load the simulation output

```
[]: data = xr.open_dataset('ch4_transport_test_out.nc')
```

6.2 Define parameters for plotting

6.2.1 Helper function for getting days and hours since simulation start from seconds

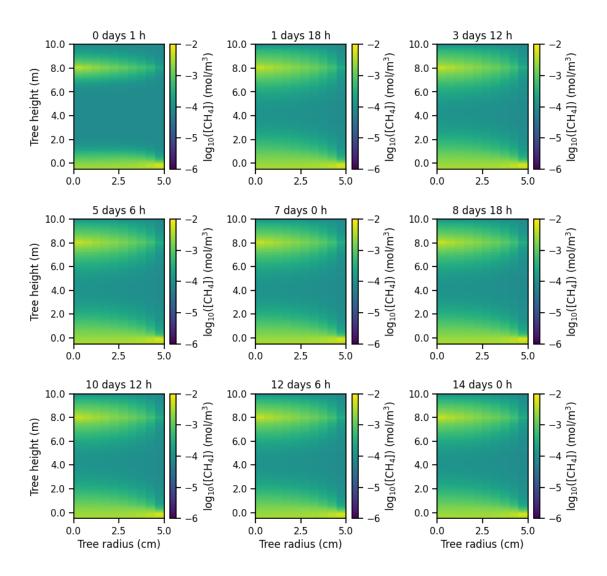
```
[]: def days_and_hours_from_seconds(seconds):
    days = np.floor(seconds/(24*60*60)).astype(np.int32)
    seconds_remaining = seconds%(24*60*60)

hours = (seconds_remaining / 3600).astype(np.int32)

return days, hours
```

6.3 Gas phase concentration at different times

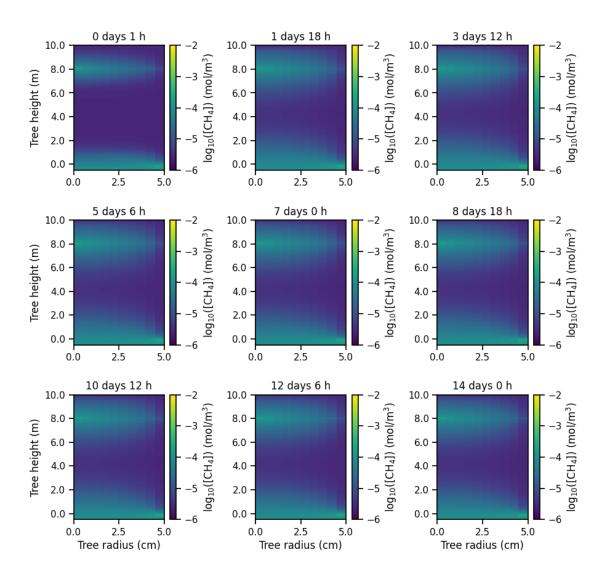
```
[]: fig, axs = plt.subplots(nrows=3, ncols=3, figsize=(10,10))
     fig.subplots_adjust(wspace=0.6, hspace=0.4)
     ind_time = np.linspace(0,simulation_time.shape[0]-2, num=9, dtype=np.int32)
     axs = axs.flatten()
     yticks = [5, 25, 45, 65, 85, 105]
     yticklabels = [f'{i:.1f}' for i in np.flip(tree_height_end)[yticks]]
     xticks = [0, 5, 10]
     xticklabels = [f'{i:.1f}' for i in tree_radius_end[xticks]]
     for i, ax in enumerate(axs):
         im = ax.pcolor(np.flipud(np.log10(data.cmp_concentration[ind_time[i], :, :, __
      →0].values)), vmin=-6, vmax=-2)
         cbar = fig.colorbar(im, ax=ax)
         cbar.set_label('log$_{10}$([CH$_4$]) (mol/m$^3$)')
         ax.set_xticks(xticks)
         ax.set_xticklabels(xticklabels)
         ax.set_yticks(yticks)
         ax.set_yticklabels(yticklabels)
         days, hours = days_and_hours_from_seconds(simulation_time[ind_time[i]+1])
         ax.set_title(f'{days} days {hours} h')
         if i in [0, 3, 6]:
             ax.set_ylabel('Tree height (m)')
         if i in [6, 7, 8]:
             ax.set_xlabel('Tree radius (cm)')
```



6.4 Aqueous phase concentration at different times

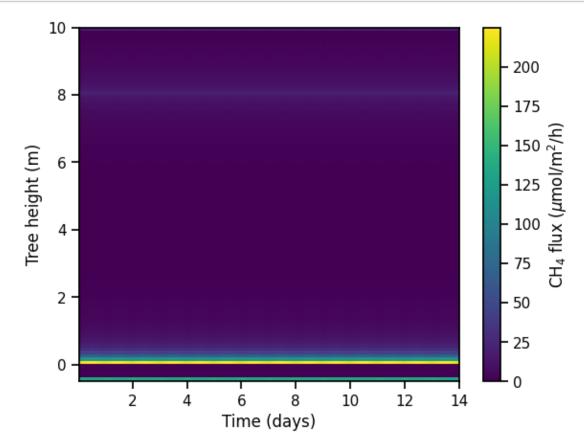
```
fig, axs = plt.subplots(nrows=3, ncols=3, figsize=(10,10))
fig.subplots_adjust(wspace=0.6, hspace=0.4)
ind_time = np.linspace(0,simulation_time.shape[0]-2, num=9, dtype=np.int32)
axs = axs.flatten()
yticks = [5, 25, 45, 65, 85, 105]
yticklabels = [f'{i:.1f}' for i in np.flip(tree_height_end)[yticks]]
```

```
xticks = [0, 5, 10]
xticklabels = [f'{i:.1f}' for i in tree_radius_end[xticks]]
for i, ax in enumerate(axs):
    im = ax.pcolor(np.flipud(np.log10(data.cmp_concentration[ind_time[i], :, :, ...)
 \hookrightarrow1].values)), vmin=-6, vmax=-2)
    cbar = fig.colorbar(im, ax=ax)
    cbar.set_label('log$_{10}$([CH$_4$]) (mol/m$^3$)')
    ax.set_xticks(xticks)
    ax.set_xticklabels(xticklabels)
    ax.set_yticks(yticks)
    ax.set_yticklabels(yticklabels)
    days, hours = days_and_hours_from_seconds(simulation_time[ind_time[i]+1])
    ax.set_title(f'{days} days {hours} h')
    if i in [0, 3, 6]:
        ax.set_ylabel('Tree height (m)')
    if i in [6, 7, 8]:
        ax.set_xlabel('Tree radius (cm)')
```



6.5 CH4 flux out of the stem

```
ax.set_xlabel('Time (days)')
cbar.set_label('CH$_4$ flux ($\mu$mol/m$^2$/h)')
```



6.6 Plot sapflow velocity and flux at 1 m height

```
fig, axs = plt.subplots(nrows=2, figsize=(8,8))
ind_1m = np.argmin(np.abs(tree_height_middle-1))
axs[0].plot(simulation_time/(24*60*60), sapflow_velocity*3600*1e2, linewidth=2,u_dcolor='steelblue')

ax2 = axs[0].twinx()
ax2.plot(simulation_time[2:]/(24*60*60), flux_out[:, ind_1m],u_dcolor='darkorange', linewidth=2)

axs[0].set_ylabel('Sapflow velocity (cm/h)')
axs[0].tick_params(axis='y', colors='steelblue')

ax2.set_ylabel('CH$_4$ flux ($\mu$mol/m$^2$/h)')
ax2.tick_params(axis='y', colors='darkorange')
```

[]: Text(0.5, 0, 'Time (days)')

