Data Set – Millennial-age GDGTs in forested mineral soils

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Soil model

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1 Soil Turnover Model

The following script estimates the turnover time of an organic compound based on its radiocarbon signature at a single point in time in different samples based on a single pool model and a two-pool model.

Define the variables here:

```
In [1]: #sampling year of the soil compound
        sampling_year = 2014

        #sample name
        sample_name = ['Bb 0-5', 'Bb 10-20', 'Bb 20-40', 'Ln 0-5', 'Ln 10-20',
                       'Ln 60-80']

        #the compound's name and its fraction modern (Fm) for each sample
        compounds = {
            'bulk':[1.007, 0.886, 0.834, 1.117, 1.015, 0.8],
            'isoGDGT': [0.964, 0.869, 0.764, 1.009, 0.821, 0.705],
            'brGDGT': [0.985, 0.851, 0.813, 0.980, 0.868, 0.595],
            'SCFA' : [0.998, 0.915, 0.934, 1.172, 1.023, 1.008],
            'C26_FA' : [0.922, 0.884, 0.768, 1.164, 0.988, 0.900],
            'C28_FA' : [0.935, 0.865, 0.731, 1.181, 1.021, 0.732],
            'Alkane' : [0.995, 0.862, 0.732, 1.141, 0.971, 0.517]
        }

        #the 2-pool-model requires an estimation of the turnover time
        #of the fast-cycling pool and an estimation of its size

        #fast turnover fraction based on the proportion of the light fraction
        #in the sample
        fast_fraction = [0.897, 0.193, 0.115, 0.162, 0.113, 0.087]

        #fast turnover based on light fraction turnover as
        #single fast pool (van der Voort, 2017)
        #fast_turnover = [354, 886, 349, 46, 236, 1181]

        #fast turnover based on SCFA single pool turnover
```

```
fast_turnover = [344, 921, 761, 33, 242, 299]

#fast turnover based on topsoil SCFA single pool turnover at all depths
#fast_turnover = [344, 344, 344, 33, 33, 33]

#the output of the two-pool model is saved as
#two_pool_turnover_{file_info}.csv
#to differentiate between tables based on different fast turnover times
file_info = 'light_fraction_turnover'
```

In [2]:
```
import math
import numpy as np
import scipy as sp
from scipy import optimize
import matplotlib as mpl
import matplotlib.pyplot as plt
import pandas as pd
%matplotlib inline
```

atmospheric CO2 data from Hua et al. (2013) and Hammer & Levin (2017)

In [3]:
```
#atmospheric CO2 Fm
#1950 - 1986 data from Hua et al. 2013
atmo_1950_1986 = [-26,-26,-26,-24,-23,17,24,98,168,280,228,219,391,827,
                  899,774,709,634,575,555,523,513,461,444,415,384,354,
                  335,324,298,272,259,241,231,213,206,193]
#1987 - 2016 data from Hammer & Levin 2017
atmo_1987_2016 = [183, 169, 158, 149, 138, 134, 126, 120, 112, 104,
                  100, 98, 90, 86.5, 80.8, 74.8, 69.1, 61.5, 57.9, 57,
                  50.1, 47.1, 46.7, 40, 38.8, 30.9,
                  22.3, 19.3, 13.4, 12.3]

atmo_1950_2016 = atmo_1950_1986 + atmo_1987_2016

#convert D14C to Fm
def D14C_Fm(D14C, year):
    return (D14C/1000+1)*math.exp((year-1950)/8267)


Fm_atmo_1950_2016 = list(map(lambda x: D14C_Fm(x[1], x[0] + 1950),
                            enumerate(atmo_1950_2016)))
```

In [4]:
```
#atmospheric CO2 Fm until sampling
Fm_atmo_model = Fm_atmo_1950_2016[:-(2016-sampling_year)]
```

Definition of Functions for single pool model

In [5]:
```
#functions
```

```
#find intial soil Fm assuming constant atmospheric Fm = 1
#before bomb testing
def find_Fini(k):
    Fini = (k/(k + 0.000121))
    return Fini

#find soil Fm of following year
def F_thisyear(k, F_lastyear, F_atmo):
    F_thisyear = k*F_atmo + F_lastyear*(1-k-0.000121)
    return F_thisyear

#find Fraction modern at the end of a list of annual atmospheric values
def F_sample(k):
    #define F_ini
    F_ini = find_Fini(k)
    #initiate for-loop
    F_lastyear = F_ini
    #for-loop
    for F_atmo in Fm_atmo_model:
        F_sample_thisyear = F_thisyear(k, F_lastyear, F_atmo)
        F_lastyear = F_sample_thisyear
    return F_sample_thisyear

#find turnover time for Fm of sample
def get_turnovertime(Fm_true):
    #loss function
    def loss(k):
        F_modelled = F_sample(k)
        return math.sqrt((Fm_true - F_modelled)** 2)
    result = sp.optimize.least_squares(loss, 0.001)
    optimal_k = result.x[0]
    turnovertime = 1/optimal_k
    return turnovertime
```

Determine the single-pool modelled turnover time for each compound at each depth and save it as a .csv

```
In [6]: Fm_samples = pd.DataFrame(compounds, index=sample_name)
        turnover_times = Fm_samples.applymap(get_turnovertime)
        pd.set_option("display.precision", 0)
        print(turnover_times)
        turnover_times.to_csv('single_pool_turnover.csv')
```

```
          Alkane  C26_FA  C28_FA  SCFA  brGDGT  bulk  isoGDGT
Bb 0-5       359     860     753   344     411   304      539
Bb 10-20    1435    1210    1403   921    1553  1190     1362
Bb 20-40    3098    2576    3113   761    1992  1743     2631
Ln 0-5        36      33      33    33     439    66      295
```

```
Ln 10-20      494      395      249    242     1372    271      1895
Ln 60-80     7779     1057     3098    299     5685   2153      3527
```

Definition of functions for two-pool model

```
In [7]: #find Fraction modern at the end of a list of annual atmospheric values
        def F_sample_2pool(k,k_fast,fraction):
            #define F_ini of slow and fast pool
            F_ini_slow = find_Fini(k)
            F_ini_fast = find_Fini(k_fast)
            #initiate for-loop
            Fslow_lastyear = F_ini_slow
            Ffast_lastyear = F_ini_fast
            #for-loop
            for F_atmo in Fm_atmo_model:
                Fslow_thisyear = F_thisyear(k, Fslow_lastyear, F_atmo)
                Ffast_thisyear = F_thisyear(k_fast, Ffast_lastyear, F_atmo)
                F_sample_thisyear = fraction*Ffast_thisyear+(1-fraction)*
                    Fslow_thisyear
                Fslow_lastyear = Fslow_thisyear
                Ffast_lastyear = Ffast_thisyear
            return F_sample_thisyear

        def get_turnovertime_combined(Fm_true, k_fast, fraction):

            #loss function
            def loss(k):
                F_modelled = F_sample_2pool(k, k_fast, fraction)
                return math.sqrt((Fm_true - F_modelled)** 2)
            result = sp.optimize.least_squares(loss, 0.001)
            optimal_k = result.x[0]
            turnovertime_slow = 1/optimal_k
            turnovertime_fast = 1/k_fast
            turnovertime = fraction * turnovertime_fast + (1-fraction) *
                turnovertime_slow
            return turnovertime

        def get_turnovertime_column(Fm_true, k_fast, fraction):
            result = []
            for i in range(len(Fm_true)):
                result.append(
                    get_turnovertime_combined(Fm_true[i], k_fast[i], fraction[i]))
            return result
```

Assuming the turnover time and the size of the labile pool the turnover time of the stabilized pool is calculated for each compound and saved as a .csv

```
In [8]: k_fast = [1/x for x in fast_turnover]
        turnover_twopool = Fm_samples.apply(
```

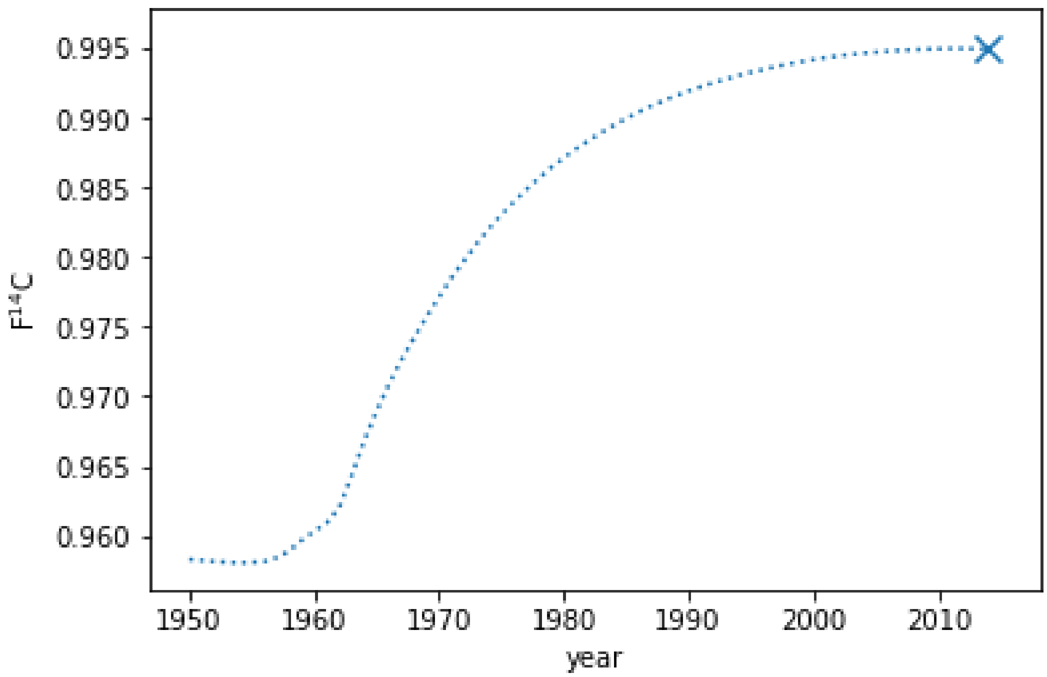
```
        lambda col: get_turnovertime_column(col, k_fast, fast_fraction))
    turnover_twopool['fast_turnover'] = fast_turnover
    turnover_twopool['fast_fraction'] = fast_fraction
    print(turnover_twopool)
    turnover_twopool.to_csv('two_pool_turnover_{}.csv'.format(file_info))
```

```
           Alkane  C26_FA  C28_FA  SCFA  brGDGT  bulk  isoGDGT  fast_turnover  \
Bb 0-5        361    2741    1669   344     446   319      739            344
Bb 10-20     1446    1214    1413   921    1569  1194     1370            921
Bb 20-40     3198    2638    3214   761    2023  1765     2697            761
Ln 0-5         36      33      33    33     547    65      357             33
Ln 10-20      503     399     249   242    1432   271     1991            242
Ln 60-80     8581    1080    3236   299    6114  2227     3700            299

          fast_fraction
Bb 0-5            9e-01
Bb 10-20          2e-01
Bb 20-40          1e-01
Ln 0-5            2e-01
Ln 10-20          1e-01
Ln 60-80          9e-02
```

plot the modelled evolution of a single sample

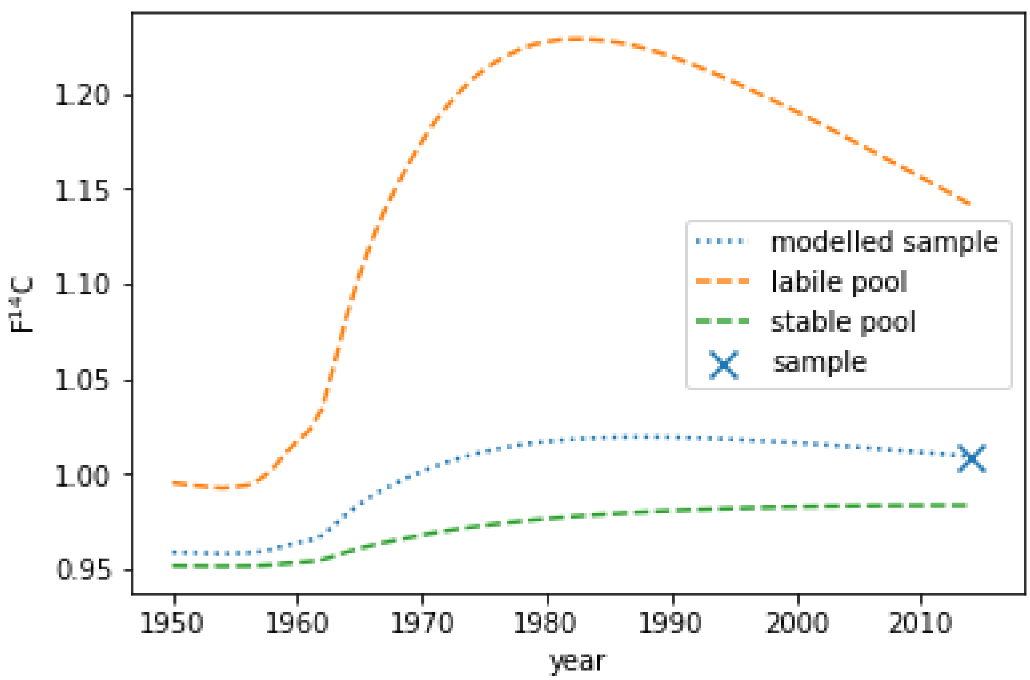
In [9]:
```
#plotting for single pool model
#enter sample D14C
Ftrue = 0.995
#enter fitted turnover time
t = 359

k=1/t

y=[]

F_lastyear = find_Fini(k)
for F_atmo in Fm_atmo_model:
        F_sample_thisyear = F_thisyear(k, F_lastyear, F_atmo)
        F_lastyear = F_sample_thisyear
        y.append(F_sample_thisyear)

x = list(range(1950, 2015))

plt.figure
plt.plot(x,y, linestyle=':')
plt.xlabel('year')
plt.ylabel('$\mathregular{F^{14}C}$')
plt.scatter(2014, Ftrue, marker = 'x', s=100)
plt.show
```

Out[9]: <function matplotlib.pyplot.show>



In [10]:
```
#plotting for two-pool model
#enter Fm of the sample, the turnover times of the labile
#and the stable pool and the fraction of the labile carbon pool
Ftrue=1.009
t_slow= 420
t_fast=33
fraction = 0.162

k=1/t_slow
k_fast=1/t_fast


y=[]
y_fast=[]
y_slow=[]

Fslow_lastyear = find_Fini(k)
Ffast_lastyear = find_Fini(k_fast)

for F_atmo in Fm_atmo_model:
        Fslow_thisyear = F_thisyear(k, Fslow_lastyear, F_atmo)
        Ffast_thisyear = F_thisyear(k_fast, Ffast_lastyear, F_atmo)
        F_sample_thisyear = fraction*Ffast_thisyear+(1-fraction)*Fslow_thi
```

```
            Fslow_lastyear = Fslow_thisyear
            Ffast_lastyear = Ffast_thisyear

            y_fast.append(Ffast_thisyear)
            y_slow.append(Fslow_thisyear)
            y.append(F_sample_thisyear)

    x = list(range(1950, 2015))

    plt.figure
    plt.plot(x, y, linestyle=':', label='modelled sample')
    plt.plot(x, y_fast,linestyle='--', label='labile pool')
    plt.plot(x, y_slow,linestyle='--', label='stable pool')
    plt.xlabel('year')
    plt.ylabel('$\mathregular{F^{14}C}$')
    plt.scatter(2014, Ftrue, marker = 'x', s=100, label='sample')
    plt.legend()
    plt.show()
```



Sensitivity of the model to assumptions

```
In [11]: #set the Fm of the sample, assumed fast turnover time and
         #the fraction of the fast pool
         Fm_true = 0.705
         t_fast = 299
         f_fast = 0.087
```

```
#set a range of fast turnover times and fractions to check
t_fast_range = range(1,799)
f_fast_range = np.linspace(0.01, 0.187, 50)

diff_t = []
diff_t_result = []
diff_f = []
diff_f_result = []
tf_ref = get_turnovertime_combined(Fm_true, 1/t_fast, f_fast)

for t in t_fast_range:
    diff_t.append((t-t_fast)/t_fast*100)
    diff_t_result.append(
        (get_turnovertime_combined(Fm_true, 1/t, f_fast)-tf_ref)
        /tf_ref*100)

for f in f_fast_range:
    diff_f.append((f-f_fast)/f_fast*100)
    diff_f_result.append(
        (get_turnovertime_combined(Fm_true, 1/t_fast, f)-tf_ref)
        /tf_ref*100)

_,axs = plt.subplots(1,2, figsize=(12,5))
plt.sca(axs[0])
plt.plot(diff_t, diff_t_result, linestyle=':')
plt.xlabel('$\Delta$ fast turnover time [%]')
plt.ylabel('$\Delta$ overall turnover time [%]')
plt.sca(axs[1])
plt.plot(diff_f, diff_f_result, linestyle=':')
plt.xlabel('$\Delta$ fast turnover fraction [%]')
plt.ylabel('$\Delta$ overall turnover time [%]')
plt.show()
```