Joseph Erbland – 15 April 2014

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TRANSITS model version 4.2 for Dome C simulation

Reference: Erbland J, Savarino J, Morin S\_, et al. Air–snow transfer of nitrate on the East Antarctic Plateau–Part 2: An isotopic model for the interpretation of deep ice-core records[J]. Atmospheric Chemistry and Physics, 2015, 15(20): 12079-12113.

Python config

* Python 3.8
* Matplotlib
* Numpy
* NetCDF4
* Scipy

Inputs :

* Time series :
  + In variable ‘input\_file\_to\_read’, e.g. “input\_time\_REALISTIC\_simulation.txt”
  + Edit in Excel

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  |  |  | **Dimensions** | |
| **Name** | **Description** | **Unit** | **Space** | **Time** |
| Accu\_mass\_rep | Mass repartition of snow accu | Adimensional | 1 | 521 |
| AT\_conc | Forced nitrate concentration in amtosphere | ngNO3-/m3 | 1 | 52 |
| AT\_height | Height of the atmospheric boundary layer | meters | 1 | 52 |
| FS\_mass\_rep | Mass repartition of the stratospheric flux | Adimensional | 1 | 52 |
| FS\_d15N | d15N in nitrate in stratospheric flux | permil | 1 | 52 |
| FS\_D17O | D17O in nitrate in stratospheric flux | permil | 1 | 52 |
| FT\_mass\_rep | Mass repartition of the long distance transport flux | Adimensional | 1 | 52 |
| FT\_d15N | d15N in nitrate in the long distance transport flux | permil | 1 | 52 |
| FT\_D17O | D17O in nitrate in the long distance transport flux | permil | 1 | 52 |
| f\_exp | Horizontally exported nitrate mass fraction | Adimensional | 1 | 52 |
| O3col\_DU | Mean ozone column in time step | DU | 1 | 52 |
| alpha | Parameter for the calculation of PSS D17O in NOx | Adimensional | 1 | 52 |
| D17O\_O3 | D17O in bulk ozone | permil | 1 | 52 |
| x\_fact | x factor for the calculation of D17O of OH | Adimensional | 1 | 52 |
| SZA\_mean\* | Mean solar zenith angle in time step | Degree | 1 | 52 |
| air\_temp\* | Mean atmospheric air temperature in time step | K | 1 | 52 |
| air\_press\* | Mean atmospheric air pressure in time step | Mbar | 1 | 52 |

\*Inputs not used in TRANSITS version 4.2  
1In the case where 52 time step per year

* File "inputs\_SZA\_rep\inputs\_SZA\_rep.txt" gives the duration in minutes spent in each degree of Solar Zenith Angle (SZA) for each time step (i.e. week in year)
  + Don’t modify this file unless working at lower latitude
* O3 photolytic rate constants stored in file "inputs\_TUV\inputs\_JO3.txt".  
  Gives the photolytic rate constant of O3 in s-1 for each time step (i.e. week in year) and for each O3 column case (i.e. 25 DU, 50 DU, …)
  + Don’t modify this file
* 14NO3- and 15NO3- photolytic rate constants stored in files such as "inputs\_TUV\inputs\_J14NO3\_0025DU.txt".  
  Gives photolytic rate constants of 14NO3- and 15NO3- in s-1
  + Modify if working with a new absorption cross section for 14NO3- and/or 15NO3-

Parameters :

|  |  |  |
| --- | --- | --- |
| **Name** | **Description** | **Unit** |
| cp\_S | Computed surface | m² |
| nb\_yr | Number of computed years | years |
| nb\_ts | Number of time steps in a year | Adimensional |
| Dt | Duration of a time step | s |
| SN\_set\_height | Height of active snowpack | m |
| SN\_set\_thick | Thickness of layers in the snowpack | m |
| SN\_d | Snow density | adimensional |
| SN\_rho | Snow volumic mass | kg/m3 |
| SN\_tau\* | Snow tortuosity | Adimensional |
| SN\_SSA\* | Surface Specific Area of snow | m2/kg |
| Phi | Photolytic quantum yield | Adimensional |
| f\_cage | Fraction of photolyzed nitrate which undergoes cage effect | Adimensional |
| D17O\_water | D17O in water | permil |
| JO3\_threshold | JO3 threshold value. For this value : 100% oxidation by OH | s-1 |
| SL\_thick | Skin layer thickness | m |
| photic\_zone | photic zone compression factor (1 is 10 cm e-folding as usual) | adimensional |
| actinic\_flux | change in the incoming actinic flux (because of solar variability or orbital parameters. Default is 1) | adimensional |
| accu\_mass\_yr | accumulated snow mass per year | kg.m-2.a-1 |
| FPI\_mass\_yr | TOTAL primary input mass deposited per year | kgN.m-2.a-1 |
| FS\_FPI\_frac | fraction of the primary input that deposits as stratospheric nitrate per year | adimensional |
| FT\_FPI\_frac | fraction of the primary input that deposits as long distance nitrate per year | adimensional |
| AT\_eps15\_dep | 15N/14N isotope fractionation at deposition of nitrate from AT to snow | permil |

\*parameters not used in TRANSITS version 4.2

Options :

|  |  |  |
| --- | --- | --- |
| **Name** | **Description** | **Unit** |
| NO2\_oxidation | Allows NO2 oxidation in atmosphere | adimensional |
| dep\_diff\_scenario | Selects the type of deposition/diffusion scenario | adimensional |
| Diff | Diff coefficient associated with dep/diff scenario number 2 | m2/s |
| O3col\_variations | Allows yearly time series of O3 column to be varied to reproduce observations | adimensional |
| sastrugi\_effect | Allows sastrugi to deposit at given time step and with a given height | adimensional |
| sastrugi\_thick | Thickness of the deposited sastrugi | meters |
| Sastrugi\_TS | Time step when the sastrugi deposits | adimensional |

* Dep/diff scenario :
  + If option.diffusion = 0 :
    - 100% of the deposited nitrate deposits to the top layers
    - No diffusion is applied
  + If option.diffusion = 1 :
    - 100% of the deposited nitrate deposits to the top layers
    - Only this deposited nitrate diffuses towards deeper layers
    - Temperature used is that of the air
    - **WARNING: turning on this option would cause unrealistic diffusion in snowpack. Suggest turning it off. -by Zhuang Jiang**
  + If option.diffusion = 2 :
    - 100% of the deposited nitrate deposits to the top layers
    - Diffusion of all the nitrate in top 1-m of the snowpack.
    - Diffusion at all time steps
    - Temperature used is that of the snow

Outputs :

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  |  |  | **Dimensions** | |
| **Name** | **Description** | **Unit** | **Space** | **Time** |
| SL\_depth | Lower depth of skin layer | meters | 1 | 521 |
| SL\_thick | Thickness of skin layer | Meters | 1 | 52 |
| SL\_mass | Nitrate mass in skin layer | kgN | 1 | 52 |
| SL\_conc | Nitrate concentration in skin layer | ngNO3-/g | 1 | 52 |
| SL\_d15N | Nitrate d15N in skin layer | Permil | 1 | 52 |
| SL\_D17O | Nitrate D17O in skin layer | permil | 1 | 52 |
| SN\_depth | Lower depth of snow layer | meters | 10002 | 52 |
| SN\_depth\_mid | Mid depth of snow layer | meters | 1000 | 52 |
| SN\_thick | Thickness of snow layer | Meters | 1000 | 52 |
| SN\_mass | Nitrate mass in snow layer | kgN | 1000 | 52 |
| SN\_conc | Nitrate concentration in snow layer | ngNO3-/g | 1000 | 52 |
| SN\_d15N | Nitrate d15N in snow layer | Permil | 1000 | 52 |
| SN\_D17O | Nitrate D17O in snow layer | permil | 1000 | 52 |
| SN\_date | Date of deposition of the snow layer | date | 1000 | 52 |
| SN\_JO3 | Photolytic rate constant of ozone at deposition of the layer | s-1 | 1000 | 52 |
| SN\_J14 | Photolytic rate constant of 14NO3- | s-1 | 1000 | 52 |
| SN\_eps15 | Photolytic 15N/14N fractionation constant | permil | 1000 | 52 |
| SN\_FP\_mass\_contri | Snow layer contribution to the photolytic flux | kgN m-2 s-1 | 1000 | 52 |
| SN\_FP\_d15N\_contri | d15N of the snow layer nitrate contributing to the photolytic flux | permil | 1000 | 52 |
| SN\_FP\_D17O\_contri | D17O of the snow layer nitrate contributing to the photolytic flux | permil | 1000 | 52 |
| FX\_mass | Mass flux X | kgN m-2 s-1 | 1 | 52 |
| FX\_d15N | d15N in flux X | permil | 1 | 52 |
| FX\_D17O | D17O in flux X | permil | 1 | 52 |
| FP\_d15N\_NOx | d15N signature of the NOx produced by photolysis (before oxidation) | permil | 1 | 52 |
| FP\_D17O\_NOx | D17O signature of the NOx produced by photolysis (before oxidation) | permil | 1 | 52 |
| AT\_mass | Mass in atmospheric box | kgN | 1 | 52 |
| AT\_d15N | d15N of atmospheric nitrate | permil | 1 | 52 |
| AT\_D17O | D17O of atmospheric nitrate | permil | 1 | 52 |
| AT\_D17O\_addO | D17O of the additional O atom in the oxidation of NO2 to form HNO3 | permil | 1 | 52 |
| AT\_D17O\_NO2\_PSS | D17O of NO2 after assuming PSS (photochemical steady state) | permil | 1 | 52 |
| FA\_mass | Mass in the archived flux per time step | kgN m-2 TS-1 | 1 | 10403 |
| FA\_d15N | d15N in the archived flux | permil | 1 | 10403 |
| FA\_D17O | D17O in the archived flux | permil | 1 | 10403 |
| FA\_thick | Thickness of the archived layer | Meters | 1 | 10403 |
| FA\_date | Date at which the archived layer was deposited at the surface | Date | 1 | 10403 |
| FA\_JO3 | JO3 in the archived layer | s-1 | 1 | 10403 |
| FA\_conc | Nitrate concentration in the archived layers | ngNO3-/g | 1 | 10403 |
| FXall\_mass | Mass flux X (over the whole computation) | kgN m-2 s-1 | 1 | 10403 |
| FXall\_d15N | d15N in flux X (over the whole computation) | permil | 1 | 10403 |
| FXall\_D17O | D17O in flux X (over the whole computation) | permil | 1 | 10403 |

1In the case where 52 time steps per year  
2In the case where snowpack is shared into 1000 layers  
3In the case where 20 years were computed (total number of time steps : 20\*52 = 1040)

Run the model :

* Single run :
  + Fill in input time series file
  + Change parameters and options
  + Fill in run01 as follows :  
    run01 = ['\_No\_sensi/',  
     ‘ ‘, 0,  
     ‘ ‘, 0,  
     ‘ ‘, 0]
  + Output NetCDF file will be stored in .\\_simulated\_data\\_No\_sensi
* Sensitivity tests runs :
  + Fill in input time series file
  + Change parameters and options
  + Uncomment the line “ set\_runs = f.Return\_list\_of\_runs('sensitivity') “
  + In functions.py, change the “Return\_list\_of\_runs” function as follows :  
    ['\_sensi\_ACCU/',  
     'accu\_mass', 75,  
     'nb\_yr', 25,  
     ' ', 0]  
    which means that the third run will be run with a snow accumulation rate of 75 kg/m2/a for a number of years of 25.
    - Up to 3 parameters can be modified at the same time
    - Output NetCDF file will be stored in .\\_simulated\_data\\_sensi\_ACCU
    - To have this case run (in this example, run03), check that runXX is in list “set\_run”
    - Not only parameters can be changed but also inputs time series or options
    - Check that the name of variable (in previous example ‘accu\_mass’ and ‘nb\_yr’) are consistent with those employed in model
* Varying ozone column time series from one year to another  
  Can be used to test McCabe’s hypothesis with observations of O3col over sevral decades
  + Run as a single run
  + Option parameter “O3col\_variations” must be set to 1
  + Fill in O3col data as in file “/inputs\_O3col/inputs\_O3col\_SP\_1978-2005.txt”
    - In this file, the first 17 years are set to the same constant time series of ozone column (observations at SP before 1967)
    - The model must be run over the 1960-2005 period, i.e. 46 years
    - Set the computation duration to 55 years and the model will be run in the 2005 conditions for another 9 years
  + If another dataset must be used, rewrite the “/inputs\_O3col/inputs\_O3col\_SP\_1978-2005.txt” file or point to another one (change the name of the file around line 31 in “model.py”)

Plot basic series when a single run has been computed :

* At end of computation and in same Python window
* Plot time series  
  Example Plot AT\_d15N versus time step number :
  + write plt.plot(out.AT\_d15N[0, :]) press enter
  + write plt.show() press enter
  + a window has opened with the plot
* Plot depth profiles  
  Example : plot d15N profile in snow at time step number 30 (in summer)
  + Write plt.plot(out.SN\_d15N[:, 30], -out.SN\_depth\_mid[:, 30]) press enter
  + Write plt.show() press enter
  + A windows has opened with the plot