Joseph Erbland – 15 April 2014

TRANSITS model version 4.2

Python config

* Python 2.7
* Matplotlib 1.1.0 for Python 2.7
* Numpy MKL 1.6.1 for Python 2.7
* NetCDF4 for Python 0.9.8
* Scipy0.12.0 for Python 2.7

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 solar zenith angle 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
  + 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-2TS-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 plot(out.AT\_d15N[0, :]) press enter
  + write 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 plot(out.SN\_d15N[:, 30], -out.SN\_depth\_mid[:, 30]) press enter
  + Write show() press enter
  + A windows has opened with the plot

MCZedits:

-1/22/2015- spin model up from 12/19 to Jan 14, roughly a month. We have BL data from 12/15, snow depth data from 12/19, and NOAA PMEL met data from 1/17. Assume constant met data before 1/17.

-1/22/2015 – changed SZA\_rep file from 52 weeks, 1 degree SZA resolution to 58 days (Dec19-Feb14), 1 degree SZA resolution. Used my MATLAB script to calculate SZA.

-1/22/2015- changed O3 column in realistic input to daily O3 at Horsepool using NASA tool: http://ozoneaq.gsfc.nasa.gov/tools/ozonemap/

-1/22/2015- In input file, changed stratosphere mass flux repartitioning to 0

-1/22/2015 – add my own temp, pressure, mean sza, wind speed, direction even though these variables are not needed.

-2/24/2015: For input\_time\_realistic\_simulation.txt file, BL NO3 concentration is from NOAA PMEL sub+super micron NO3- concentration measurements. Ozone from NASA tools. Mean SZA from NOAA SZA calculator (this is mean SZA during time I was digging snowpit (typically from 10-2). Air temperature, pressure, wind speed, and wind direction from NOAA PMEL met data. Boundary layer height from Bill Neff measurements at Horsepool.

-2/24/2015- The O3 used will be the mean ozone from the input file, not the O3 text file inputs, because the O3 text files are for comparing many different years (1960 to 2005)

-3/9/2015 – The x-factor is used to calculate D17OH and is the ratio of the net loss with respect to the total loss (isotopic exchange reaction term + net chemical loss term). From Morin et al., 2007, at lower latitudes, the x-factor is nearly zero (Michalski et al., 2003). **Change from 0.5 to 0 here**.

-3/9/2015 – The alpha, or A, factor described the PSS NO2 ratio, which is the equation in Alexander et al. 2009, and Morin et al., 2007, Savarino et al., 2009. It is the ratio of NO2 production via NO+O3 /NO+HO2, NO+RO2, etc. Typically is 0.8 in day and 0.95 at night. I change to 0.7 to because there are lots of HO2 and RO2 in Uintah Basin.

-3/9/2015 – Parameters to vary: horizontally exported nitrate mass fraction, cage effect, long distance repartition, diffusion coefficient, vary NO3 concentrations between PMEL and hi-vol value

-3/9/2015 – Plan: spin-up model to first snow pit (1/15/2014). Iterate then from snowpit to snowpit, using the j values from the previous snowpit.Deposit 20 cm at the very start and then for on 1/30, deposit 5 more cm.

-3/12/2015 – For “tuv” actinic flux files, I use METCON data from Hans Ostoff for January 22nd and February 4th as two representative days. For every SZA (50-90), I average 10 second increments of radiation data together for every wavelength from 280.5-350 (in increments of 0.5 nm). Then I add up the two half wavelengths to get integer wavelengths (e.g. 280, 281). I use the values from 290 for wavelengths less than 290. For wavelengths greater than 345, I use the 345 radiation data. Then I convert W/m2\*nm units to photons/cm^2\*s by multiplying the W/m^2\*nm value by (5.03E11 \* (lambda, in nm) / 1.42). The 5.03E11 \* lambda part comes from [www.berthold.com/en/bio/how-do-i-convert-irradiance-photon-flux](http://www.berthold.com/en/bio/how-do-i-convert-irradiance-photon-flux), and the 1.42 comes from the factor Hans Ostoff told me to divide all the data by because of some measurement error.

-3/12/2015- For now, I calculate the actinic flux at each value (from surface to 19 cm) as Finc (from above) \* 3.831 \* exp(-0.6\*k\*z), assuming an exponential decay. The k is the effective cweff from my 2013 paper, that takes into account Kext and cweff. For those, I used just approximate values in the middle range of all values measured from this campaign.

-3/12/2015 – The original deposition rate I used was 0.03 cm/s from GEOS-Chem, but now try using lower 1-1.5 cm/s value from the Edwards paper 2013 paper. But change to 0.02 cm/s because it agrees much better with observations and also is what is reported for dry deposition of O3 in Edwards et al., 2014 (HNO3 is very reactive, like O3).

-3/12/2015 – for accumulation rate, it freaks out if it’s zero, so I put it to 0.001, both for the total amount of accumulation, but also for the amount to repartition each day.

-3/12/2015 – in input\_file, got D17O and d15N (long-distance), from average of all atmospheric d15N over campaign.

-3/12/2015 –Depth of each pit: pit 1=18 cm, pit 2 = 9 cm, pit 3= 14 cm, pit 4 = 18 cm, pit 5 = 11 cm, pit 6 = 18 cm, pit 7 = 20 cm, pit 8 = 15 cm, pit 9 = 14 cm, pit 10 = 24 cm, pit 11 = 21 cm, pit 12 = 20 cm

-3/12/2015 – Because each snow pit has variable depths, make radiation files of different lengths for each snowpit. Then spin up each pit from the start (12/19) to the date of the pit, using the pit depth of each pit from the start. Then view d15N and NO3 profiles. Once there is accumulation on 1/31, spin up like normal, then add 5 cm of snow to it on last day. Then calculate profiles. WOOT!

-3/14/2015 – Even though have two actinic flux datasets (1/22 and 2/4), use the 1/22 for all snowpits just to see change in snow optical properties. Perhaps later, use the actinic flux value for each day to be more exact.

-3/16/2015 – There doesn’t appear to be much diffusion in the snow, either use the average of all snowpit bottom NO3 values to initialize (291.2), or force the model with the lowest NO3 value for each snowpit (341.9 for pit 1, 390.6 for pit 2, 538.3 for pit 3, 197.1 for pit 4, 613 for pit 5, 494.9 for pit 6, 185.6 for pit 7, 142.9 for pit 8, 144.9 for pit 9, 162.8 for pit 10, 195 for pit 11, 1072.4 for pit 12.

-3/16/2015 - The cage effect changes the amount of NOx fluxed from the snow. If cage effect = 1, FNOx is 0. Fraction exported influences surface NO3 and d15N (top few cm), so we should try to estimate this now. Highest FNOx when 0 is exported, so keep this as an upper limit for now.

-3/16/2015 – **changing the diffusion timestep does nothing! Does not speed up diffusion.**

-3/17/2015- Looked at the NO3 and d15N for all snowpits. Some of them look pretty good, but in others, the NO3 concentrations are too low. Play with diffusion I guess, but I don’t understand where Joseph got his x10^-11 value from. From my diffusion coefficients, I keep calculating 10^-6 values.

-4/6/2015 – Using new version (v50) from Joseph. Need JNO2.txt file in inputs\_tuvfolder

-4/6/2015- I think I want the compression factor to be 1. I want full depth of snowpit in photic zone

-4/6/2015 – I need to get concentrations of all BrO, CO, CH4, RH, HO2, CH3O2, but really just BrO for now. Do others later because they seem optional.

-4/6/2015 – get relative humidity too (from NOAA PMEL ACG). It has a wide variation over the course of the campaign – from 45 to 90%. Take 70% as a good average.

-4/6/2015- for atmospheric ozone, use max from each day of campaign and then use campaign average to fill in pre-campaign values.

-4/21/2015- modified the input\_time\_REALISTIC\_simulation in two ways. The atmosphere d15N is now (in input\_time\_...SNd15N), the value of d15N at the snow surface for each different day of the campaign, using the previous snowpit value until getting to the next snowpit. To spin the model up, the average surface d15N measurement is the average of surface values from pit 1-8 (7.3).

-4/21/2015- the input\_time\_REALISTIC\_simulation (no new ending) has been modified to be the air d15N value for that day. Before the campaign when there is no data, the average campaign value is still used. Use average d15N value (9.3) whenever there is no atmospheric d15N data. If there are 2 d15N measurements for one day, use the d15N for the day when the filter was taken off.

-4/21/2015 – make the changes to d15N in the input file first, then think about changing the amount of NO3 deposited for each snowpit. For now, don’t mess with changing the amount of NO3 deposited. Right now, it’s using the average PMEL NO3- data with a specific deposition rate for the length of the simulation (divvy-ed up to deposit an equal amount of NO3- each day).

-4/22/2015 – change D17O initial condition to 30, based on rough average from bottom of all snowpits.Also change d15N initial condition to be 1.5, which is average of bottom value for all snowpits. Potentially use individual d15N values for each snowpit later.

-9/13/2015 – EMAIL FROM JOSEPH ABOUT UPDATING MODEL TO HAVE INITIAL VERTICAL PROFILE

I have worked on the model initialization. Please, replace the "functions.py" by the attached one ("functions.pyc" will be updated automatically once you run the model).

Also, please copy/paste the attached "initial\_snow\_conditions.xlsx" file at the same level as the main file.

In "initial\_snow\_conditions.xlsx", you want to place the data (conc, d15N, D17O) for the initial snowpack. Please, use the same layering as used in the model (+ one last layer which is necessary for the model to work - I can explain you why if you want but it is not important. In this last layer, just copy/paste the values for the one above and increase the depth by 1 cm).

You can see that there is a tab for each snowpit in the "initial\_snow\_conditions.xlsx" file. Please create new tabs for the other pits. The selection of the data for each pit is done in "functions.py" at line 188.

Important note : in "functions.py", line 136, there was a mistake which could have caused some problems when you used the model.

It was originally written :  
self.SN\_final\_nb = int(1/self.SN\_set\_thick)

(whichimplicitely assumes that the modeled snowpack height is 1 meter)

It now reads :  
self.SN\_final\_nb = int(self.SN\_set\_height/self.SN\_set\_thick)

From your files, I can see that you had to find some "tricks" when setting the value for SN\_set\_height (line 366 in main). For example "pit11=21 cm (try 16 cm)". Why is that?

This may have been caused by my mistake above.

I have to confess that I don't entirely understand how you used the model. In several places, I have the feeling that some of your choices were not appropriate and I acknowledge that your task here is difficult since this modeled was designed for snow several meters thick where we only look at what happens in the top layer (in my case, the top meter) and record what gets archived.

Here is a suggestion : what about a skype in the coming days (or whenever is best for you) to check at every step what you did with the model so that I could assist you efficiently?

I prefer to work in this way rather than getting back and forth by email.

One last thing : you can get rid of the "\_simulated\_data" folder which contains by old runs outputs and must be useless to you.

Also, I wonder how you extract the model outputs so that you can use them to draw some plots.

dfdf