PTloop2.0 userguide (MATLAB version)

Alice Vho, July 2020

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Get started

1. Be sure that you have MATLAB (2015b or more recent) and Theriak installed. Theriak package available at: https://titan.minpet.unibas.ch/minpet/theriak/theruser.html.
2. Download and unzip the folders named "PTloop" and "WorkingDirectory" in Documents/MATLAB/.
3. Run MATLAB.
4. Select the folder “PTloop” as current folder in MATLAB (the window “Current Folder” should look like Fig. 1).
5. Run the installer (right click on "Install_PTloop.p" > run).
6. Follow the instructions (Figures 3-5). You will need to provide the folder were Theriak is located.

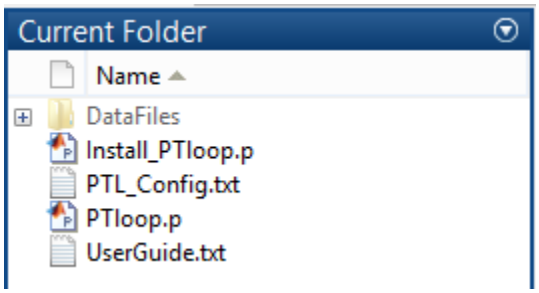

Figure 1.

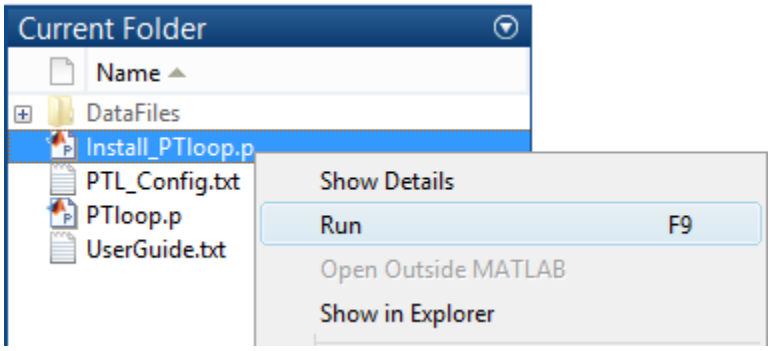

Figure 2.

Figure 3.

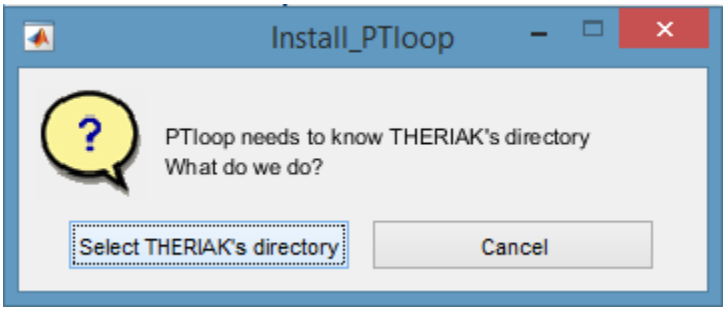

Figure 4.

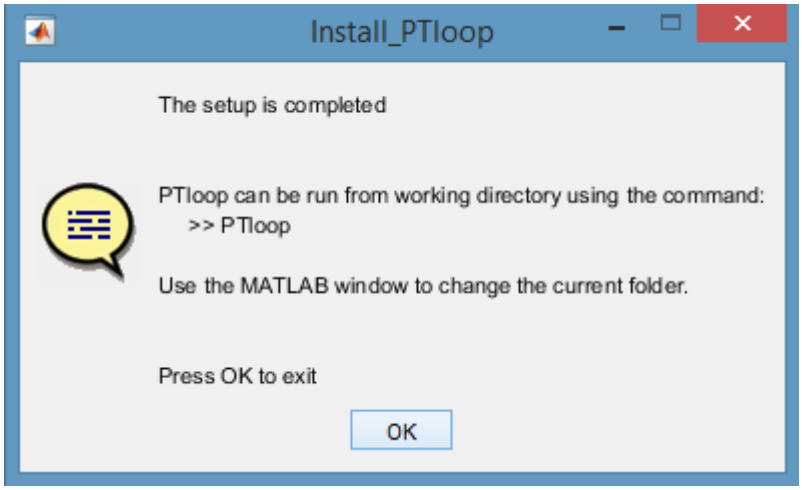

Figure 5.

Parameter setting

1. Make sure that the folder containing the main program (PTloop.p) is added to your MATLAB path (Fig. 6).
2. Navigate with MATLAB to your WorkingDirectory (Fig. 7). This folder contains the following files:
   - theriak.ini (Theriak file for thermodynamic modelling)
   - PTlin.txt (input file for PTloop calculations)
   - Fluid_in.txt (input file for infiltration of external fluid)
   - Fluid_out (output file with the information of the released fluid)
   - DBOXYGEN oxygen isotope fractionation database
   - One (or more) thermodynamic database(s)
   - For each thermodynamic database please make sure that in the folder PTloop/DataFiles the corresponding "SSModel_[NameDatabase].txt" file is present. This file is fundamental for linking the thermodynamic and the oxygen isotope fractionation databases. If you want to add a new database, you will need to create an associate SSModel file (see section "Create/modify an SSModel file).

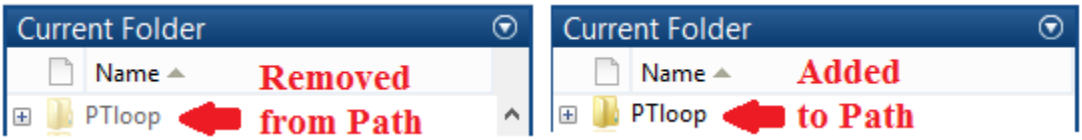

Figure 6.

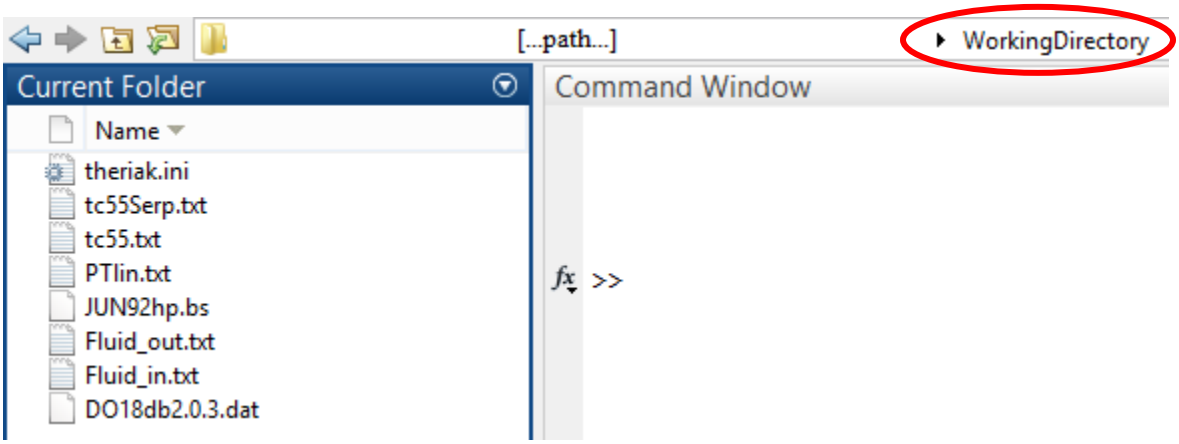

Figure 7.

3. Open the file PTlin.txt and set the desired input parameters. For the details on each parameter, see supplements to the publication Vho, Lanari, Rubatto and Hermann (2020), Tracing fluid transfers in subduction zones: an integrated thermodynamic and $\delta^{18}O$ fractionation modelling approach, Solid Earth, doi.org/10.5194/se-11-307-2020.
4. Save and close the file.
5. Open the file Fluid_in.txt and set the PT, amount and $\delta^{18}O$ of the external fluid (for no external fluid, set the mass to 0 kg). The number of P-T steps must correspond to those set in the PTlin.txt file. If you are not sure how many steps and at which P-T conditions you set, run PTloop (point 1 of section "Calculate") and count how many points are displayed in the P-T path. If you still have doubts, read the point 1 in the section "Good to know!" below.
6. Save and close the file. Now you are ready to perform the corrected calculation with the desired amount of external fluid.

Calculate

1. Run PTloop by typing in the MATLAB Command Window "PTloop" and pressing Enter. The PTloop working window will appear (Fig. 8).

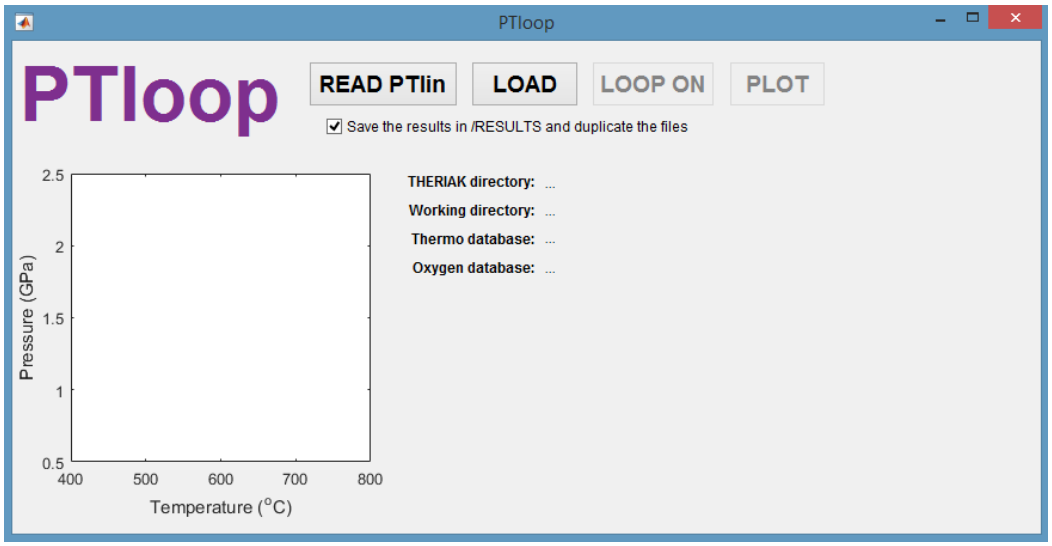

Figure 8.

2. Make sure that the option "Save the results" is selected if you want your results to be saved.
3. Press "READ PTlin". The defined P-T path and additional parameters are shown (Fig. 9). If you want to modify anything, open the file PTlin.txt, modify it, save it, close it and press again "READ PTlin".

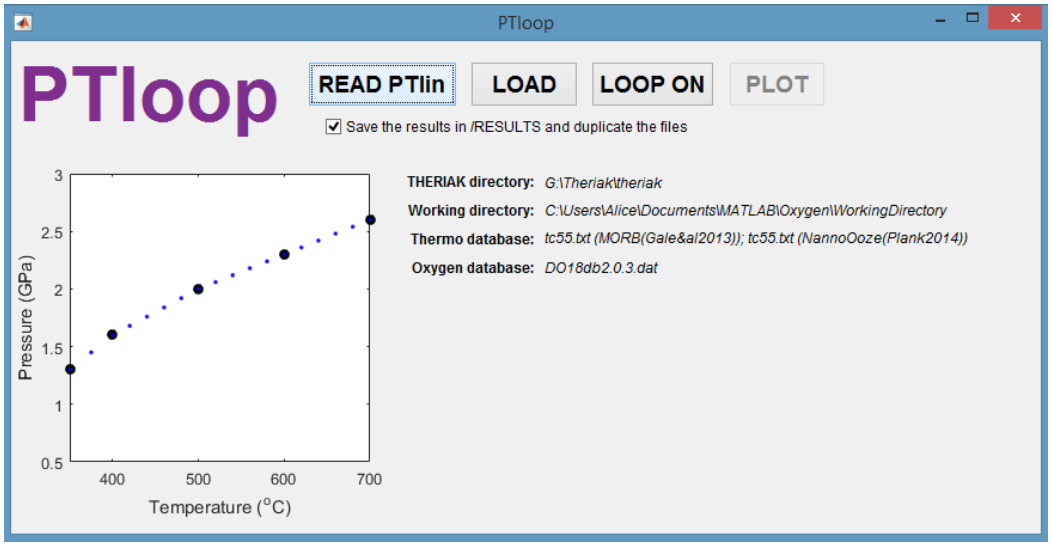

Figure 9.

4. Press "LOOP ON".
5. A folder "RESULTS" will be created and all the result files, as well as all the version of the databases that have been used for the calculation and the input files, will be saved. All the details are displayed in the MATLAB command window and are saved in the file "Printout.txt" automatically created in the folder RESULTS.

Reading the results

Results are saved in the folder "RESULTS" (1) in a graphical format (subfolder Figures) and (2) in a MATLAB file (named RESULTS_PTloop.mat) that can be re-opened at every time by double clicking on it. In addition, the Printout.txt file contains all the information displayed in the MATLAB Command window during the simulation and the file "Fluid_out.txt" contains the P, T, mass (kg) and $\delta^{18}O$ of the fluid released by the whole system at each step.

Figures

Nine different figures are created, each one both as MATLAB figure and as pdf file.

- FIG_0_d18OvsFluidWt%: $\delta^{18}O$ of the total fluid released by the system (left axis) and released fluid wt% of total rock (right axis)
- FIG_0_d18OvsTotalMassFluid: $\delta^{18}O$ of the total fluid released by the system (left axis) and released fluid mass in kg (right axis)
- FIG_0_Fluids
  Panel 1: Mass of fluid (kg) released by rock1 (continuous black line), released by rock2 (dashed black line) and transferred from rock1 to rock2 (red line)
  Panel 2: $\delta^{18}O$ of the fluid released by rock1 (continuous black line), released by rock2 (dashed black line) and released by the whole system (blue line)
  Panel 3: Fluid/rock ratio (mass/mass) in rock2
- FIG_1_d18O: $\delta^{18}O$ of the stable mineral phase and of the excess fluid at each step in rock1
- FIG_1_ModeBox: Volume fraction of stable phases in rock1
- FIG_1_VolFrac: Volume fraction of stable phases in rock1
- FIG_2_d18O: $\delta^{18}O$ of the stable mineral phase and of the excess fluid at each step in rock2
- FIG_2_ModeBox: Volume fraction of stable phases in rock2
- FIG_2_VolFrac: Volume fraction of stable phases in rock2

In all the plots but the modeboxes lines are shown, meaning that if a phase (solid/fluid) occurs only at one step of the simulation (and not at the previous and at the following ones), it will not be represented. The same applies for the fluid released by each rock type and by the whole system. If a single fluid pulse occurs, its magnitude and the isotopic composition of the fluid will not be plotted; however, it will be reported in the results (file "RESULTS_PTloop.mat" , see below).

Quantitative results

The detailed results are contained in the MATLAB file RESULTS_PTloop.mat available in the "RESULTS" folder. To load this file, double click on the file name in the "RESULTS" folder. Make sure that the "Current folder" is the "RESULTS" folder. In alternative, type in the MATLAB command window "load('RESULT_PTloop.mat')" (Fig. 10) and press Enter. The file will appear as variable in the Workspace. Double click on it to open it (Fig. 11).

Figure 10.

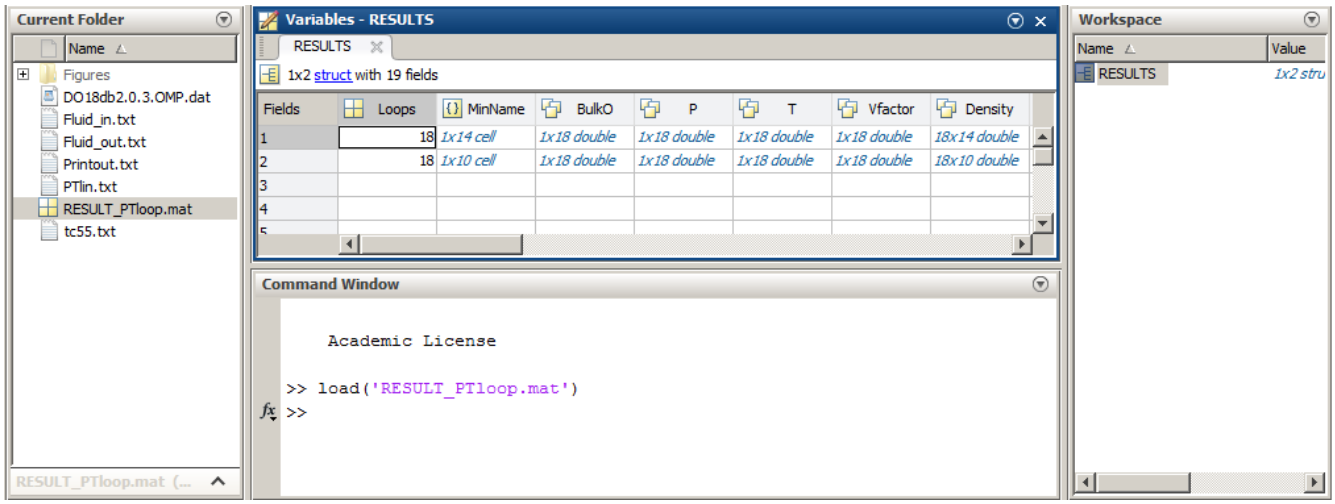

Figure 11.

The RESULTS variable is composed of two rows; the first row refers to the results for Rock1 and the second row to results for Rock2. In the following, all the components are explained. To open each sub-variable, double click on the cell of interest.

- Loops: number of loops
- MinName: List of all the phases that appear in the rock assemblage along the simulation (named as in thermodynamic database)
- BulkO: bulk $\delta^{18}O$ at each step
- P: pressure (bar) at each step
- T: temperature (°C) at each step
- Vfactor: the volume of the rock might change along the P-T path. This value reports the volume at each step as fraction of the initial volume
- Density: density of each phase at each step (kg/dm3). Each column corresponds to one phase (see MinName) and each row to a step. When a phase is not stable, the reported density is 0
- Volume: volume of each phase at each step as reported in Theriak output (ccm)
- VolumePer: volume fraction of solids (as reported in Theriak output divided by 100)

- VolumeFrac: volume fraction of each phase (columns) at each step (rows) normalized to 1
- IsFractionated: it indicates weather a phase has been fractionated from the reactive bulk (1) or not (0) at each step
- dO18: $\delta^{18}O$ of each phase at each step
- RealVolFrac: volume fraction of each phase at each step not normalized to 1
- MassOfFluidInKgPer1Kg: mass of external fluid entering the rock at each step in kg of fluid per kg of rock
- MassOfFluidOutSystemTotalKg: mass of fluid (kg) that are leaving the system from each rock type at each step
- dO18_FluidOut: $\delta^{18}O$ of the fluid leaving the rock at each step

CHECK: contains some additional information.

AR/AI = after reacting/after input (i.e. with the incoming fluid). BR = before reacting (i.e. with the incoming fluid).

- AR_MassMineralsFractionated: mass (kg) of the phase fractionated at each step
- AR_MassFluidsFractionated: mass (kg) of the total fluid released by the system
- BR_MassFluidInTotalKg: mass (kg) of external fluid entering rock1 at each step (as defined in the file Fluid_in.txt) or in rock2 at each step (as released by rock1 and controlled by the chosen degree of interaction)
- AR_MassRockKGPer1KG: mass of rock with respect to the initial mass at each step (i.e. accounting for the loss of fluid)
- AR_ReactiveMassOfRockTotalKg: mass (kg) of the reactive rock at each step (i.e. accounting for the loss of fluid and fractionated minerals)
- AI_MassRockKGPer1KG: mass of rock with respect to the initial mass at each step considering that in rock1 the initial mass includes the first input of fluid (i.e. occurring at step1)

Good to know!

1. The Fluid_in.txt file works based on the number of lines: every line corresponds to the fluid the infiltrate the system at each step, i.e. line 2 to step 1 (line 1 being the header), line 3 to step 2, and so on. If the P and T conditions are not precise, do not worry: the fluid will be anyway let infiltrate at the precise P-T conditions of each step calculated by PTloop based on the PTlin.txt file. For instance, if step 4 of your calculation is at P = 23450 bar and T = 473 °C and at line 5 of the file Fluid_in.txt you write P = 23500 bar and 470 °C (or 3 bar and 10 °C, or any values), the fluid will still infiltrate the rock at P = 23450 bar and T = 473 °C.
2. At every calculation, the program replaces all the files in the RESULTS folder. If you are interested in keeping your previous results, just rename the folder. A warning is active to remind you this!
3. PTloop can perform calculations only in one direction, meaning that a combination of prograde and retrograde path cannot be set (T and P can only increase or decrease). If a retrograde path is defined,

the final figures will appear with increasing T from left to right, therefore they must be read from right to left. The .pdf file can be easily modified with any suitable program by flipping vertical the plot.

4. If you like to used a modified version of the provided thermodynamic databases, you might face some issues, such as phases/solid solutions that are not present in the SSModel file. You can create a new SSModel file (or modify an existing one) by following the instructions in the section "Create/modify a SSModel file".
5. If you notice a white field in the ModeBox figure, most likely a phase/solid solution is missing in the SSModel you are using. Run a Theriak simulation at the P and T of interest and compare the phase assemblage with the PTloop result to understand which mineral is missing. You can create a new SSModel file (or modify an existing one) by following the instructions in the section "Create/modify a SSModel file".
6. There is a maximum water content that is supported by the program and depends on the Theriak output format. The program can deal with a THERIN having a maximum of 999.9999 moles of H (Fig. 12). Above this value, an error will occur (in the Command Window of MATLAB you will read in red "Undefined function or variable 'VOL_Names'). This occurs because in the Theriak output some numbers have no more space between each other (Fig. 13) and cannot be read correctly.

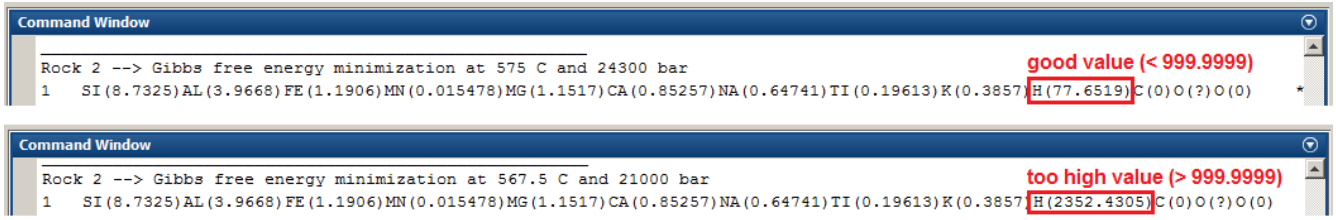

Figure 12.

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elements in stable phases:
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```

	O	AL	CA	FE	H	K	MN	MG	NA	SI	TI	E
GARNET_alm	5.353149	0.892191	0.253778	0.856661	0.000000	0.000000	0.015279	0.212570	0.000000	1.338287	0.000000	0.000000
CHTD_fctd	1.196502	0.341858	0.000000	0.099408	0.341858	0.000000	0.000199	0.071322	0.000000	0.170929	0.000000	0.000000
PHNG_mu	5.095186	1.049546	0.000000	0.030368	0.849198	0.385700	0.000000	0.081758	0.038899	1.385922	0.000000	0.000000
ClAMP_gl2	7.394992	0.553945	0.034162	0.204163	0.616249	0.000000	0.000000	0.786051	0.608511	2.463659	0.000000	0.000000
lawsonite	5.646304	1.129261	0.564630	0.000000	2.258521	0.000000	0.000000	0.000000	0.000000	1.129261	0.000000	0.000000
quartz	4.488884	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	2.244442	0.000000	0.000000
rutile	0.392260	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.196130	0.000000
water.fluid	1174.182337	0.000000	0.000000	0.0000002348.364674		0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
total:	1203.749613	3.966800	0.852570	1.1906002352.430500		0.385700	0.015478	1.151700	0.647410	8.732500	0.196130	0.000000

Figure 13.

Create/modify a SSModel file

The SSModel files located in the folder "PTloop > DataFiles" (Fig. 1) contains the key for the interaction between a thermodynamic database and an oxygen isotope database. As any of this is modified or new

versions are available, it is necessary to update the existing SSModel files or even create new ones. Luckily this is an easy task, and you can create your own SSModel file that suits your modified database!

Structure of a SSModel file

First of all, the SSModel file must be named correctly. The name must be "SSModel_[name of the thermodynamic database].txt. For instance, for tc55.txt, the SSModel file name is "SSModel_tc55.txt.txt".

The internal structure of the file is divided into 2 parts: the solid solutions (Fig. 14) and the pure phases (Fig. 15). For the solid solutions (SS), the structure is the following. Nb. O = number of oxygen as reported in the thermodynamic database.

```
>> COMMON NAME OF THE SS          NAME OF THE SS IN THE THERIAK OUTPUT
    COMPONENT1*     COMPONENT2*     COMPONENT3*     ....
    component1**    component2**    component3**    ....
    Nb. O comp.1    Nb. O comp.2    Nb. O comp.3    ....
```

* as present in the oxygen isotope fractionation database
** as present in the thermodynamic database

```
*** SOLID SOLUTIONS ***

>> OLIVINE      OLIVINEi
FAYALITE        FORSTERITE
fayalite        forsterite
4               4

>> CARBONATE    CCDO
CALCITE         MAGNESITE       DOLOMITE
calcite2        magnesite2      dolomite2
6               6               6

>> FELDSPAR     FSP
ALBITE          ANORTHITE       KFELDSPAR
high-albite     anorthiteC1     sanidine
8               8               8

>> ILMENITE     ILM
ILMENITE
Oilmenite
3
```

Figure 14.

For pure phases, the structure is the following:

```
NAME IN THE DBOxygen DATABASE    NAME IN THE THERMODYNAMIC DATABASE    Nb.O
```

```
*** MINERAL DATA ***
CLINOHUMITE              clinohumite              18
ANDRADITE                andradite                12
ANDALUSITE               andalusite               5
KYANITE                  kyanite                  5
SILLIMANITE              sillimanite              5
ZOISITE                  zoisite                  13
ZOISITE                  clinozoisite             13
EPIDOTE                  Fe-epidote               13
EPIDOTE                  epidote                  13
LAWSONITE                lawsonite                10
TITANITE                 sphene                   5
ZIRCON                   zircon                   4
```

Figure 15.

Modify a SSModel file

In order to add a new pure phase, it is enough to add a row at the block named ***MINERAL DATA*** by respecting the structure defined above. In order to add a new solid solution, leave an empty row below the previous block, then create a block following the structure explained above, and add an empty row between the created block and the following one. If you want to remove a block, you can (1) cancel it or (2) add an exclamation point (Fig. 16) as first character of each row of the block. In this way the block is just deactivated, meaning the you can reactivate it by removing the exclamation points at any moment you need it again.

```
!>> EPIDOTE              EPI
!ZOISITE                 EPIDOTE
!clinozoisite            Fe-epidote
!13                      13
```

Figure 16.