CZGM-iso

The CZGM (Compositional Zoning in Garnet and its Modification by diffusion) software models the initial compositional profiles in garnet and their modification by diffusion as function of time and temperature during metamorphism.

Its published version (Faryad and Ježek, 2019, Lithos, 332-333, 287-295**) uses fractionation computed by the program Vertex (**Connolly, 2005**).**

The CZGM-iso is simplified version, which creates the garnet profiles from isopleths provided by Vertex as the output files from Werami. Fractionation is neglected.

Presentation by example

The example for demonstration of the CZGM-iso is about garnet from metapelite in garnet zone, where no diffusion of the initial profiles occurred.

This includes selection of a PT path and definition of a garnet size distribution population generated based on the compositional and volume isopleths.

The calculated compositional profiles of individual garnets are compared with the measured profiles in garnet.

Some examples from two stages and high-grade metamorphic rocks are also shown.

Software installation and data preparation

The software works under MATLAB.

After installation of MATLAB, copy and unzip the CZGM-iso.zip file on your PC.

The GZGM-has two folders: CODE & DATA. Files in the CODE folder should not be changed by the user. In DATA folder some files must be prepared:

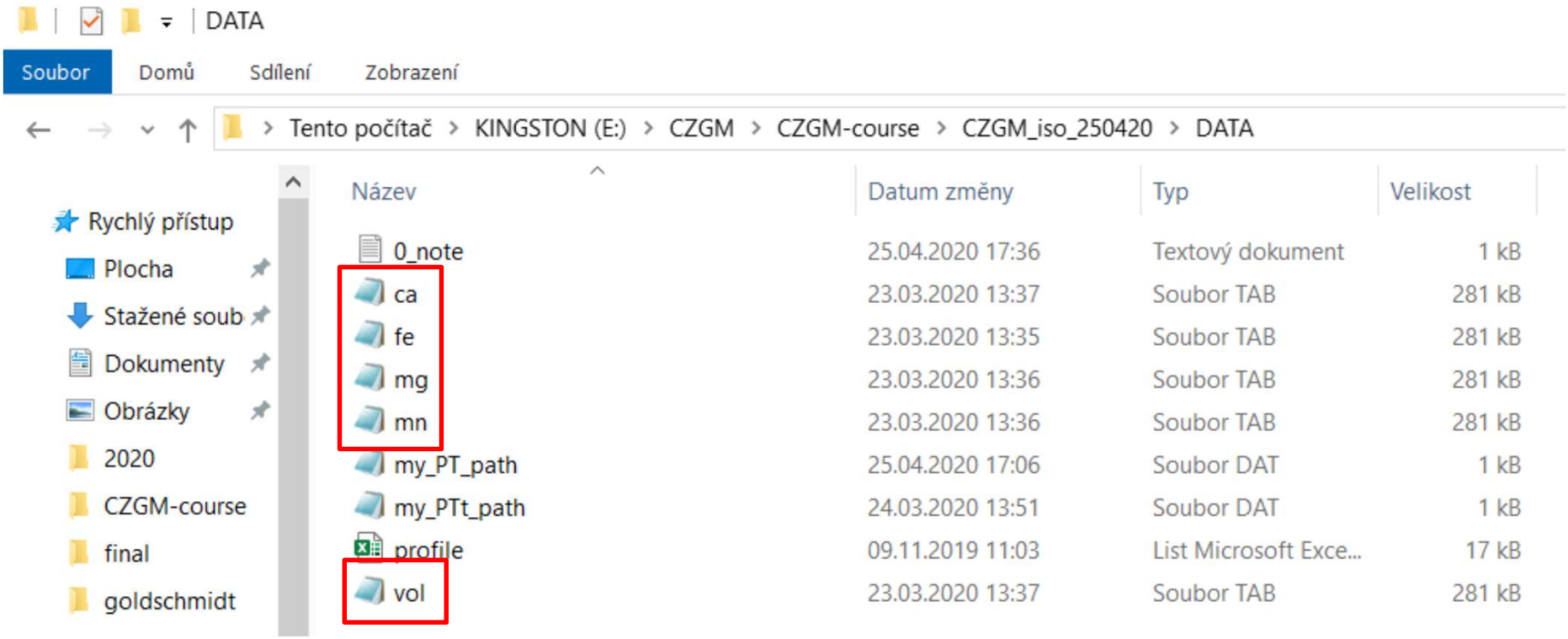
After calculation of pseudosection using Vertex (version 2019), compositional isopleths for garnet should be calculated using Werami.

To compare the results of calculated and measured data, compositional profiles in measured garnet are needed to tabulate in an Excel sheet.

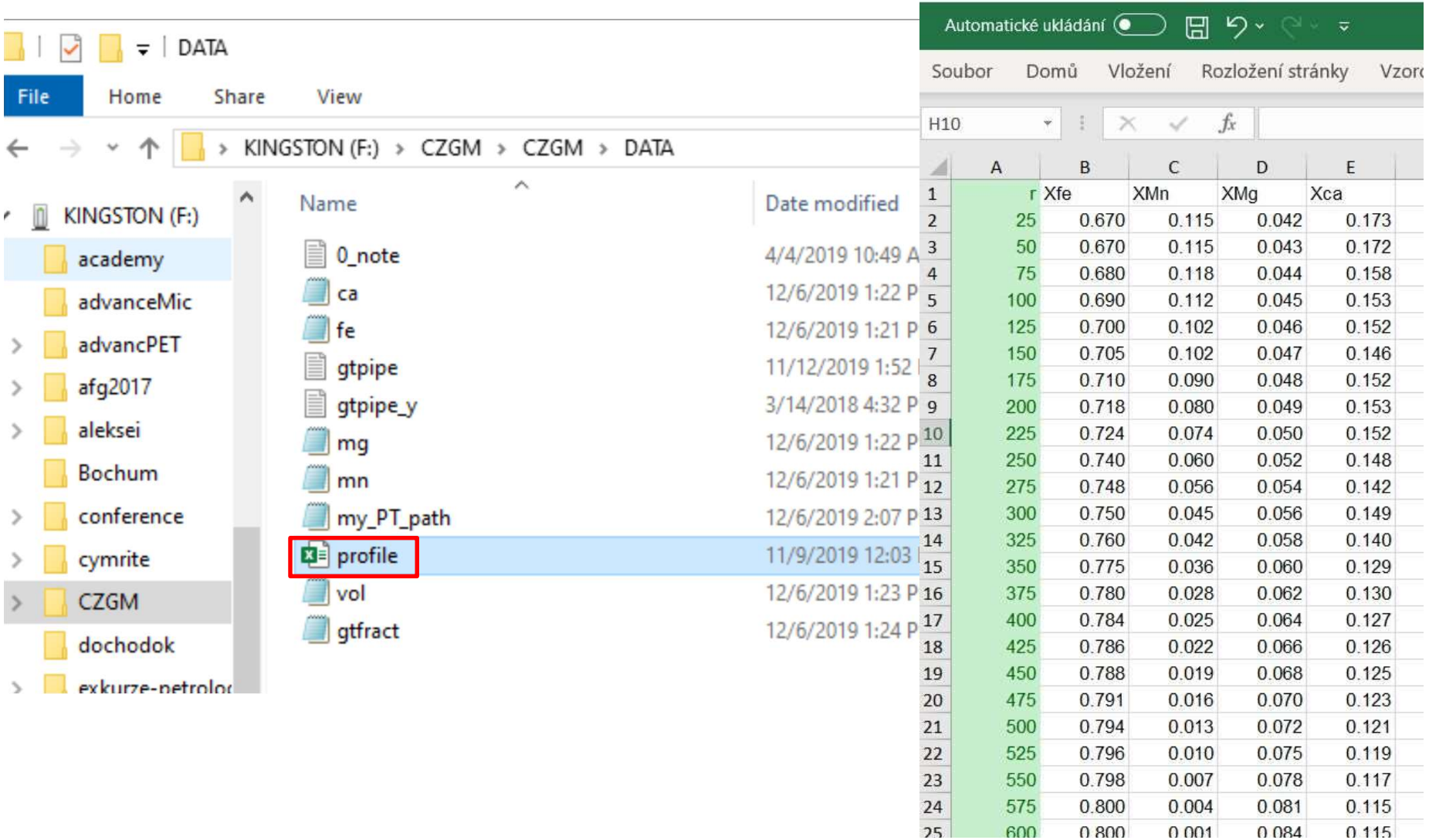
(In comparison to the published CZGM-vertex version, there is no need to add any Vertex files to CODE.)

The DATA folder contains:
isopleths of Fe, Mn, Mg, Ca vol % of garnet calculated using Vertex and Werami (version 2019).

They are in the files: **fe.tab** **mn.tab** **mg.tab** **ca.tab** **vol.tab**



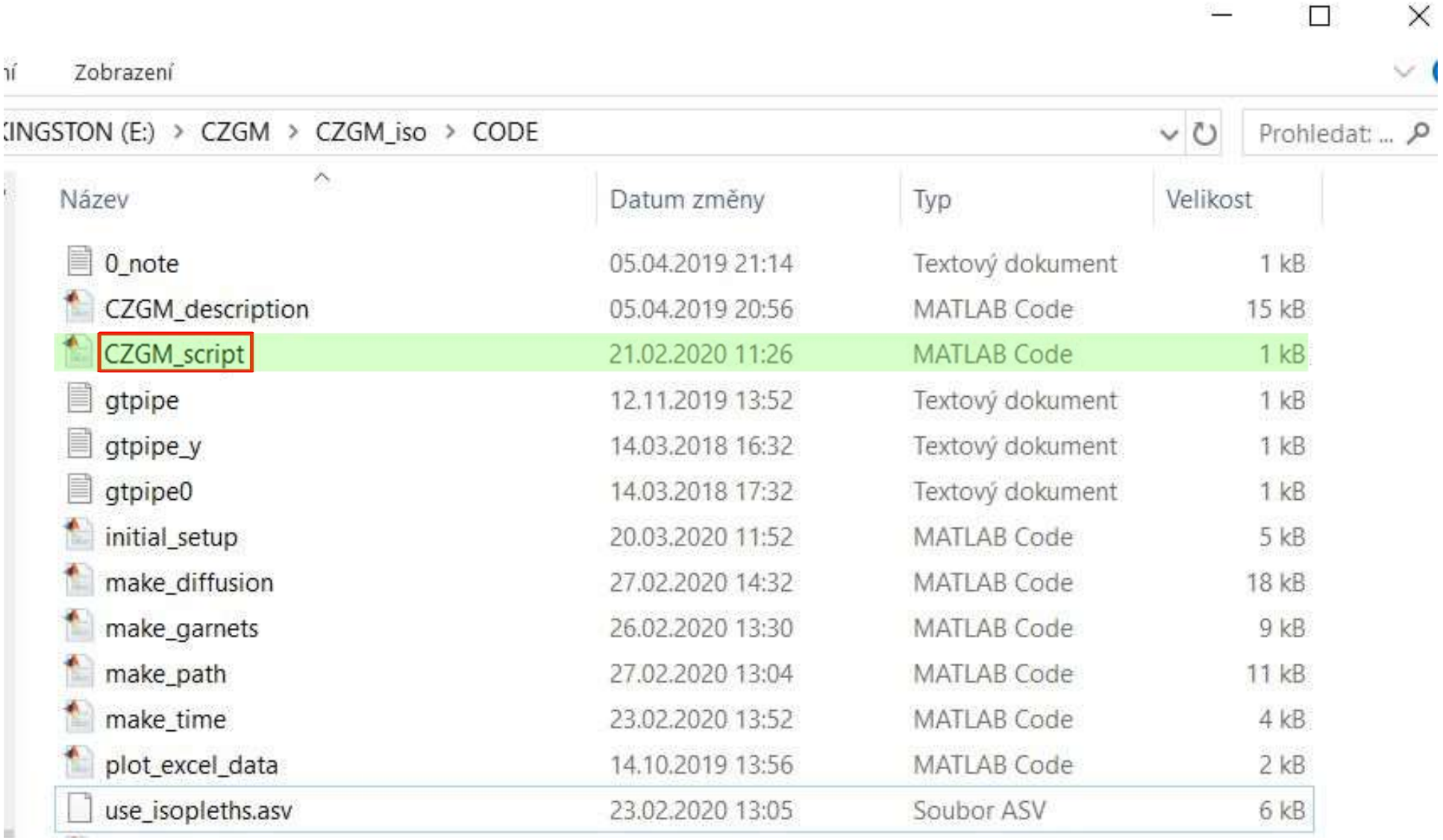
In order to compare the modelled garnet profiles with the measured ones, the measured data can be tabulated in an Excel: sheet r-radius (in microns), X_{Fe}, X_{Mn}, X_{Mg}, X_{Ca}.
Call it as profile.xlsx and save it in the DATA folder.



	A	B	C	D	E
1	r	Xfe	XMn	XMg	Xca
2	25	0.670	0.115	0.042	0.173
3	50	0.670	0.115	0.043	0.172
4	75	0.680	0.118	0.044	0.158
5	100	0.690	0.112	0.045	0.153
6	125	0.700	0.102	0.046	0.152
7	150	0.705	0.102	0.047	0.146
8	175	0.710	0.090	0.048	0.152
9	200	0.718	0.080	0.049	0.153
10	225	0.724	0.074	0.050	0.152
11	250	0.740	0.060	0.052	0.148
12	275	0.748	0.056	0.054	0.142
13	300	0.750	0.045	0.056	0.149
14	325	0.760	0.042	0.058	0.140
15	350	0.775	0.036	0.060	0.129
16	375	0.780	0.028	0.062	0.130
17	400	0.784	0.025	0.064	0.127
18	425	0.786	0.022	0.066	0.126
19	450	0.788	0.019	0.068	0.125
20	475	0.791	0.016	0.070	0.123
21	500	0.794	0.013	0.072	0.121
22	525	0.796	0.010	0.075	0.119
23	550	0.798	0.007	0.078	0.117
24	575	0.800	0.004	0.081	0.115
25	600	0.800	0.001	0.084	0.115

Starting Matlab and CZGM

Run Matlab, set work directory to CODE and open CZGM_script.m.
Or go to the CODE folder and click on the CZGM_script.

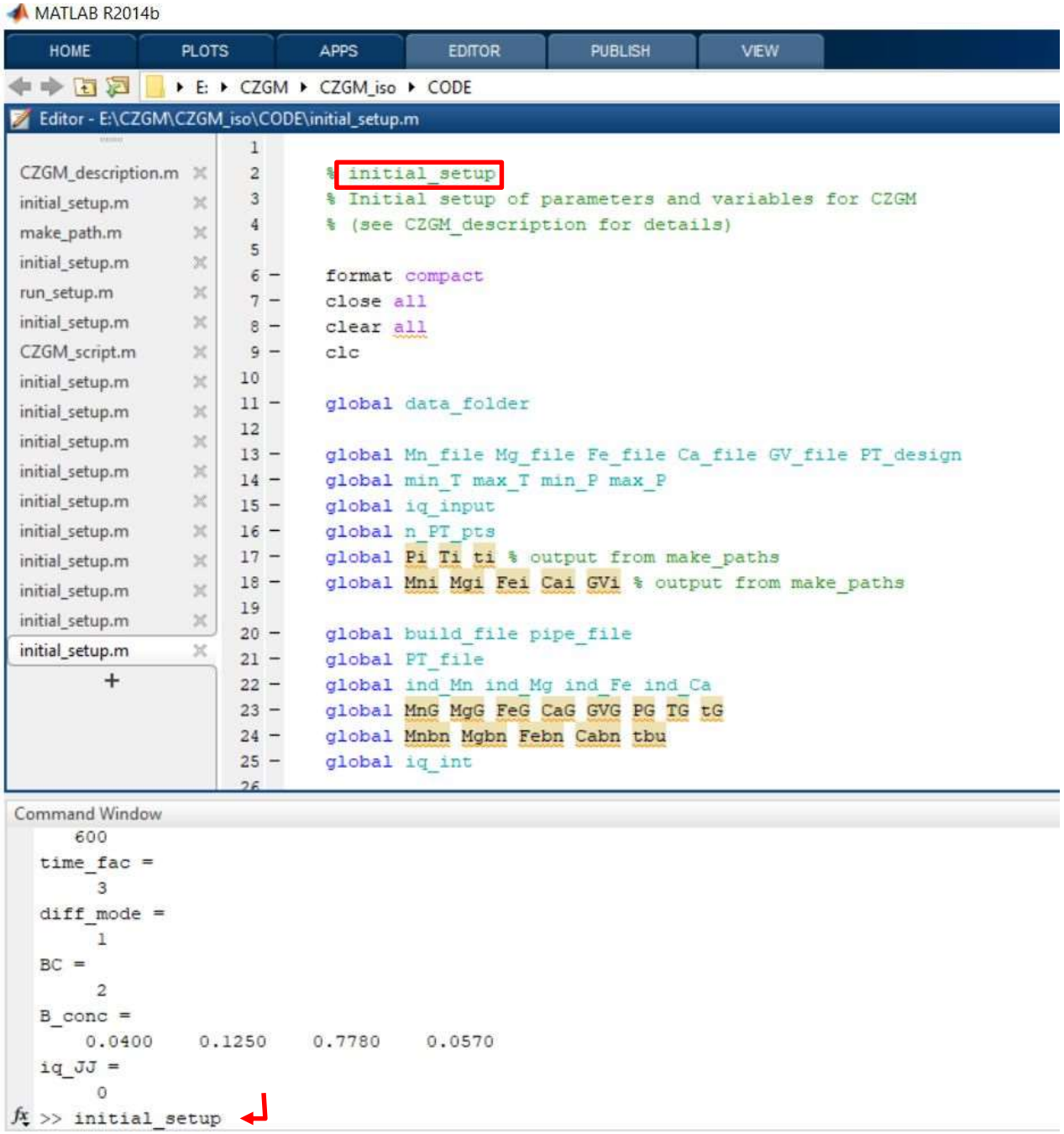


Modelling sequence

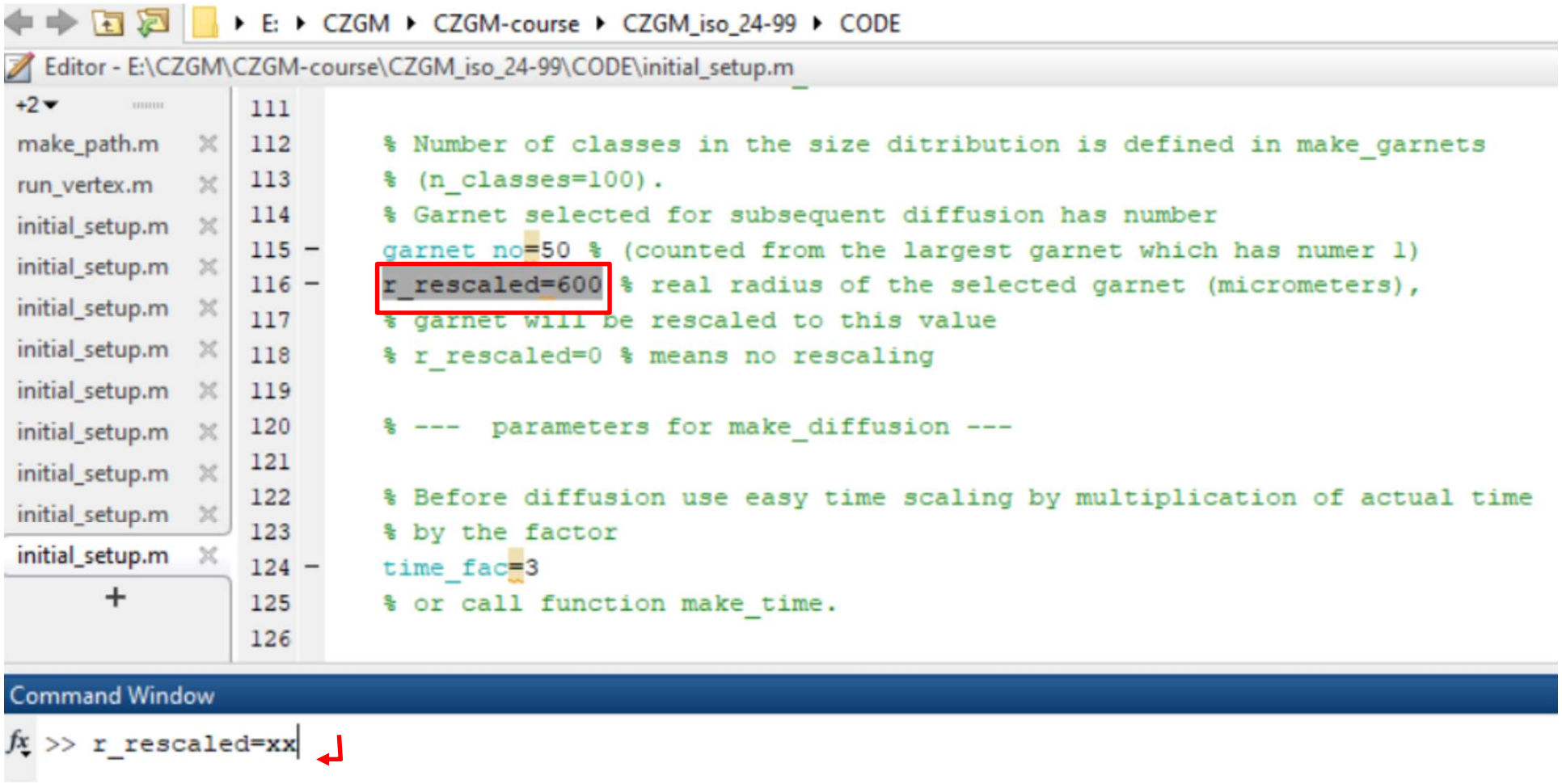
Modelling sequence is described in the file CZGM_script.m

```
 % (0) Preparation and initial setup
initial_setup
 % (1) Design of PT-path
make_path
 % (2) Gathering material for garnets
use_isopleths
 % (3) Formation of garnet population
make_garnets
 % (5) Multicomponent diffusion in a chosen garnet
make_diffusion
```

Run intial_setup

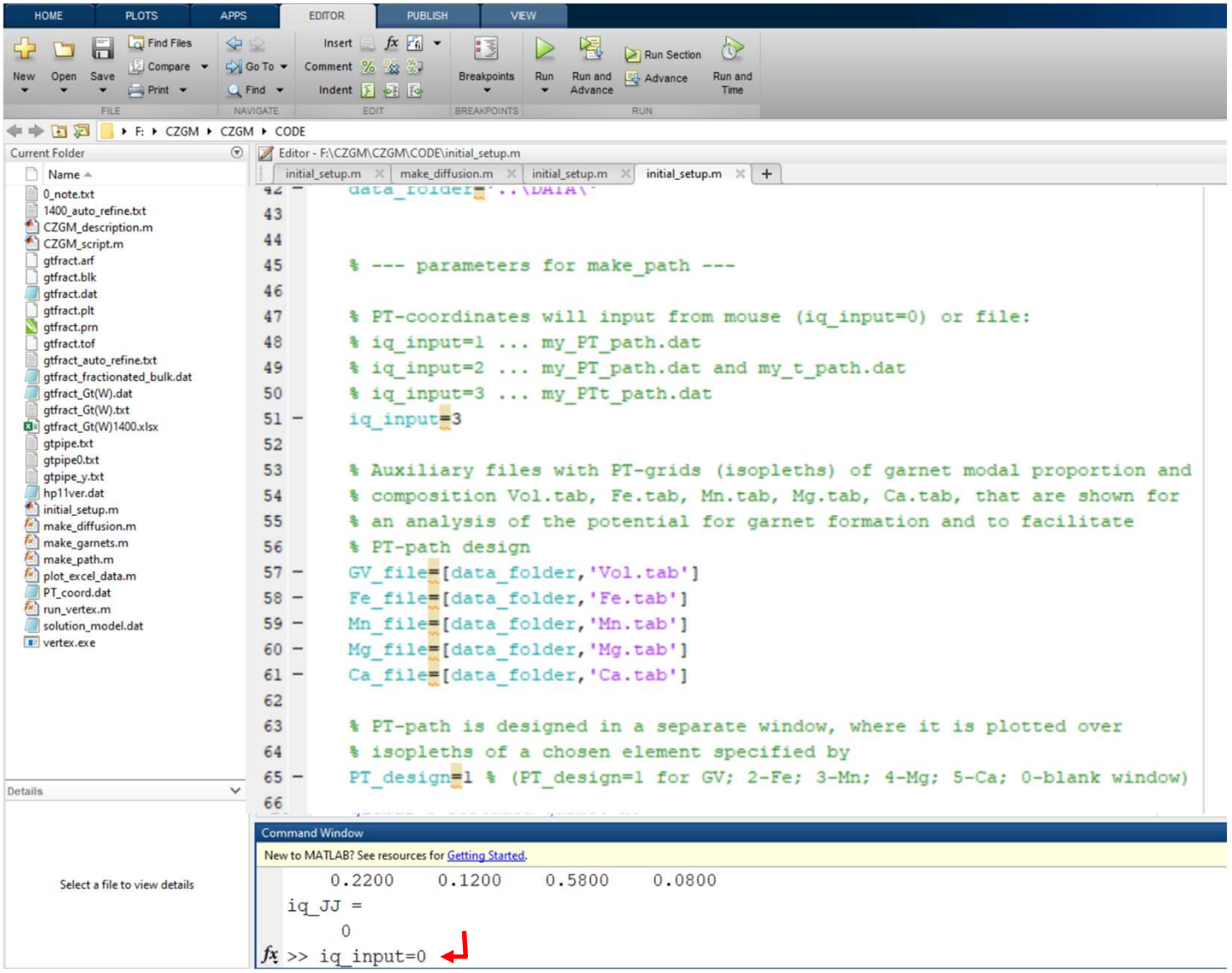


All parameters for CZGM are pre-defined by running initial_setup. They can be changed afterwards from command line. For example, if the garnet radius is not correctly specified, it can be defined by adding the value by command : r_rescaled=xx (real size in micrometers)

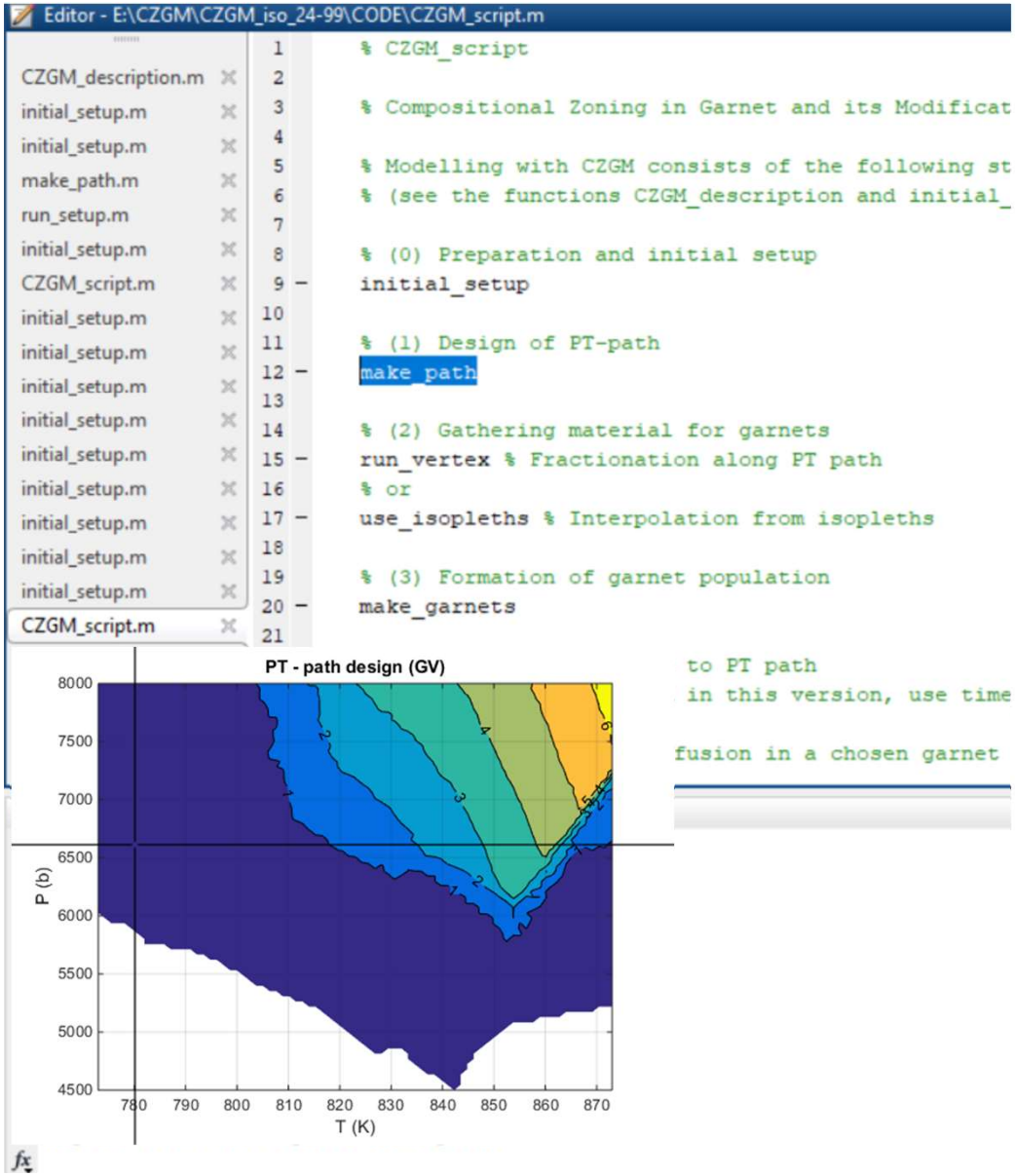


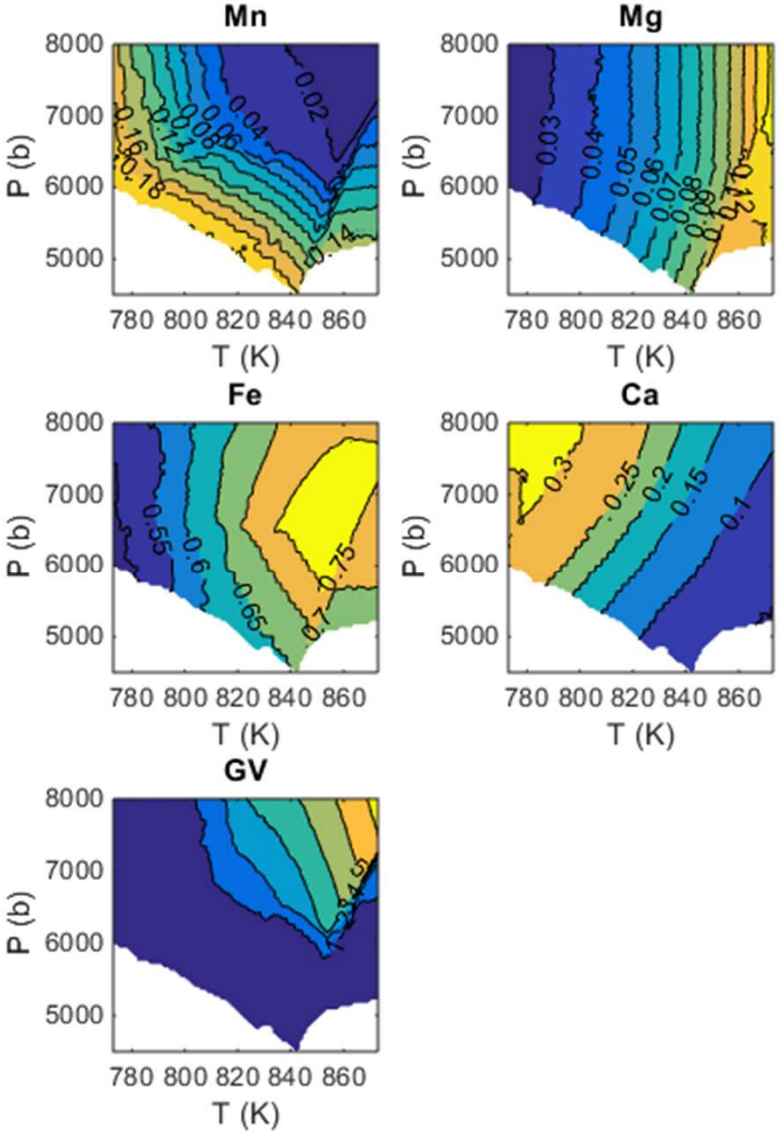
Step 1: make_path

For iq_input=0, the PT path will be defined by hand (mouse).
Set this from command line and run make_path.

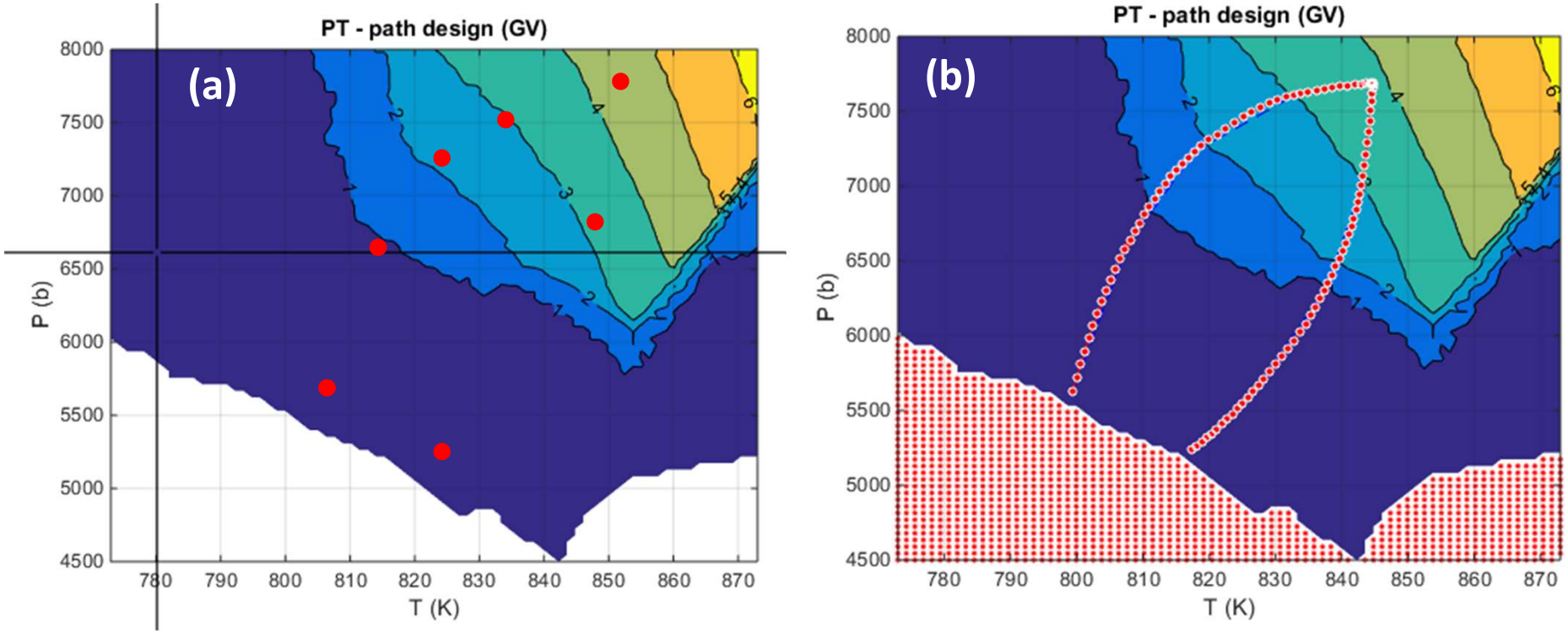


The function will draw isopleths prepared by Werami and allow you to set the PT path in one of the windows.

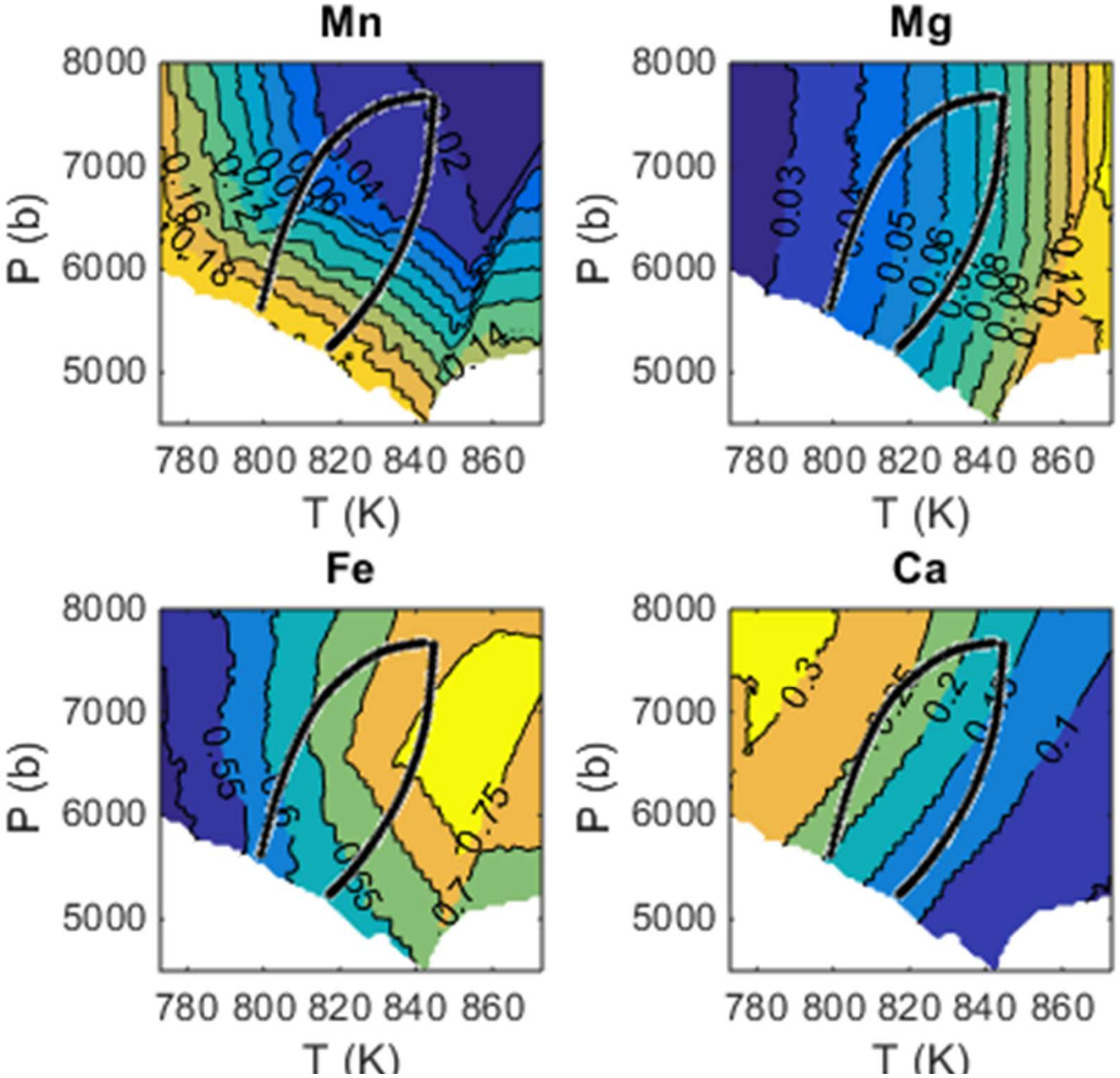




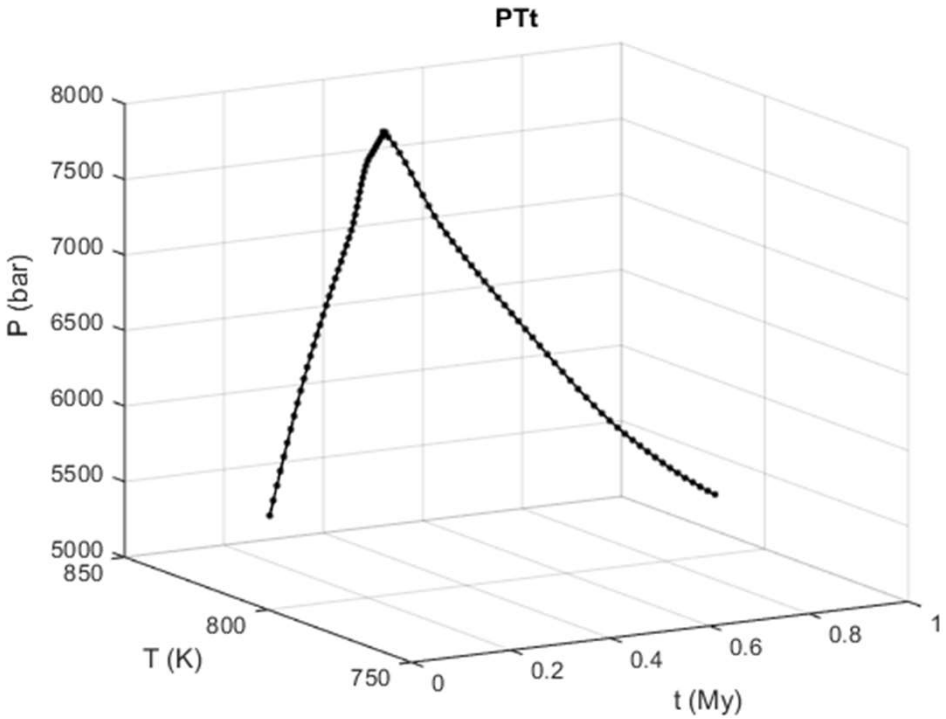
Constraining PT path by hand:
The image of garnet volume content (GV) is selected to draw the PT path. By clicking the left mouse button you will select points on the PT grid and by clicking the right button you will end the PT path (Fig. a). The program will automatically connect the selected points and draw the PT path (Fig. b).

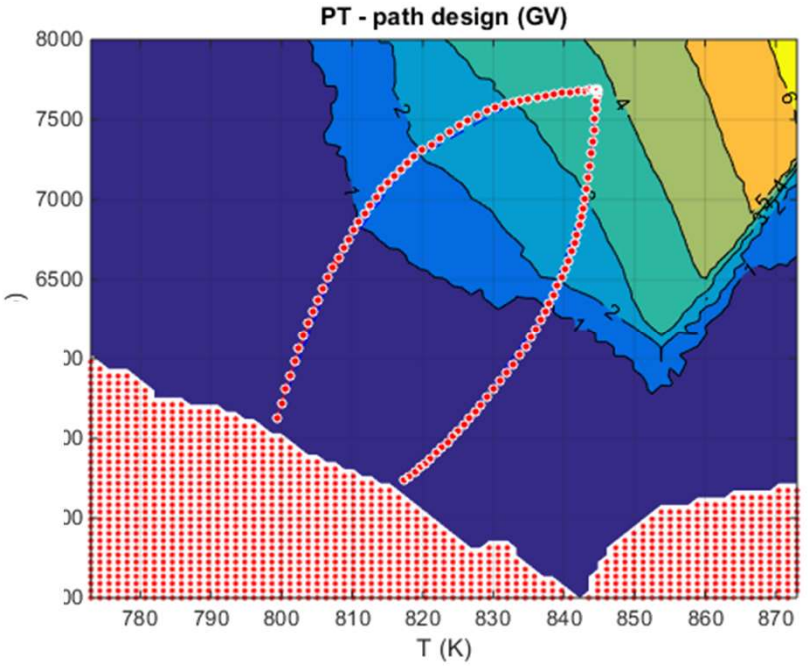


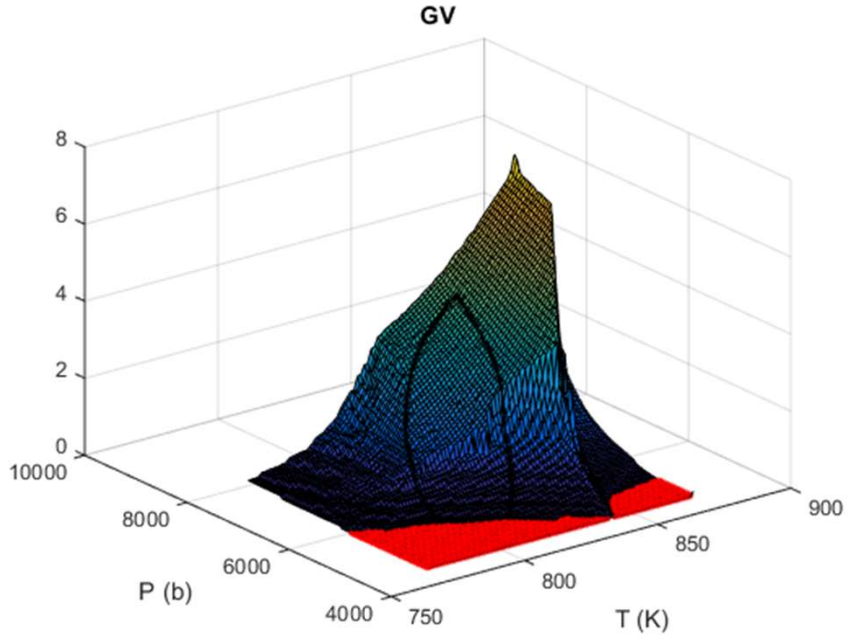
The PT paths will appear also on the compositional isopleth diagrams.



Additional illustrating figures about the PT-t and PT-GV offered by the program:

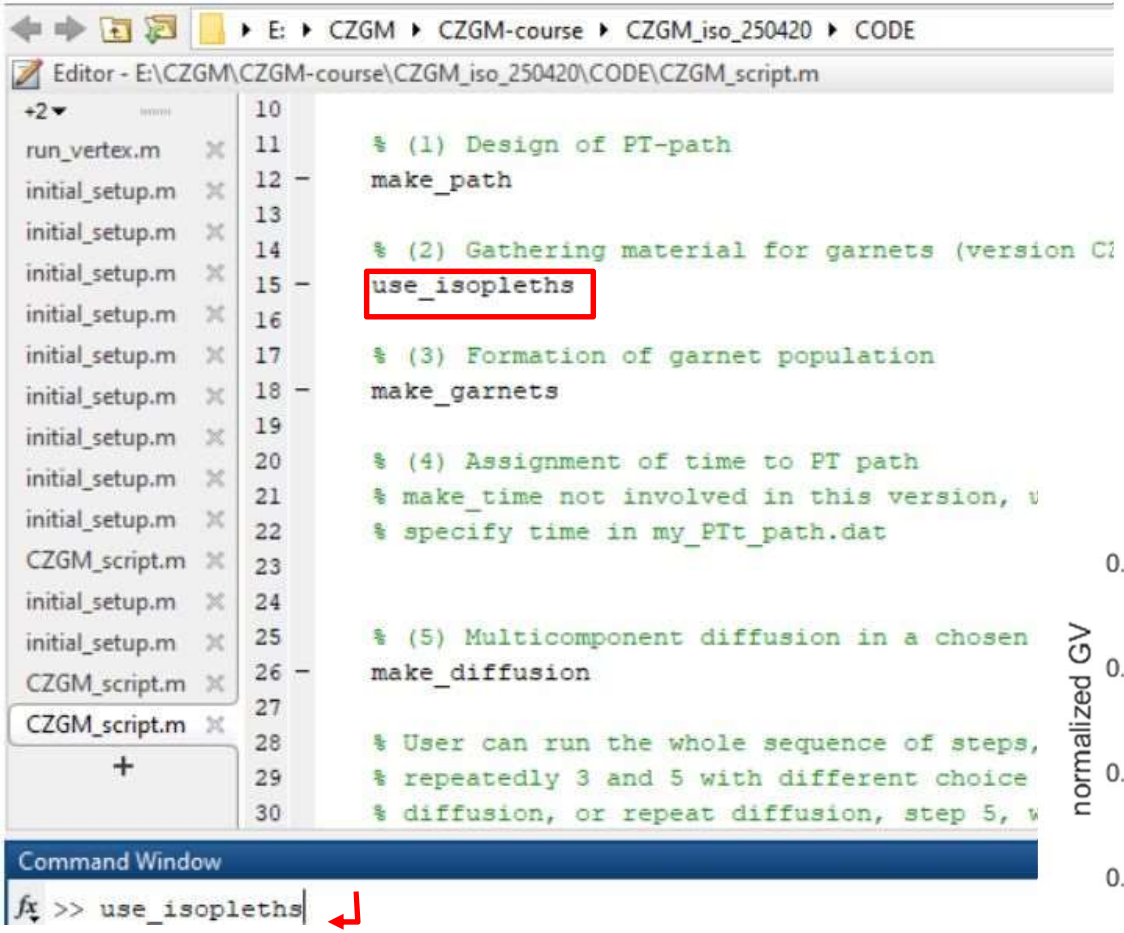


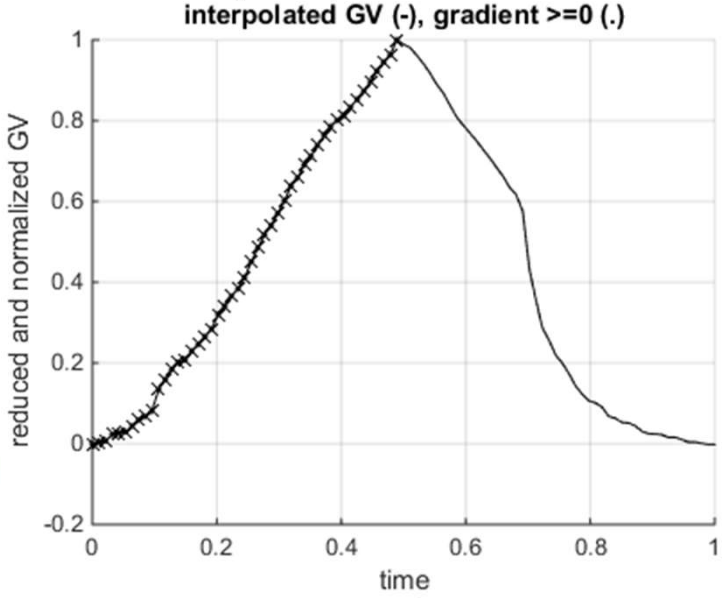


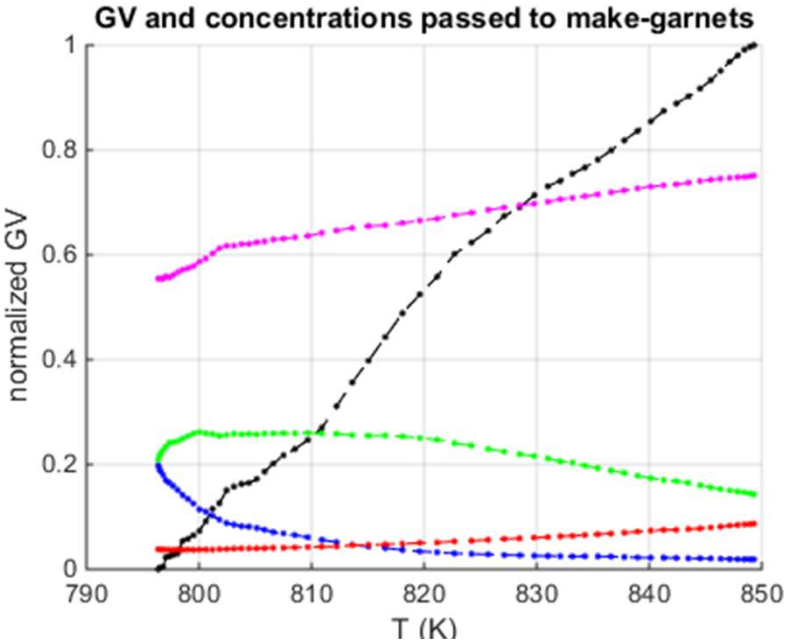


Step 2: use_isopleths

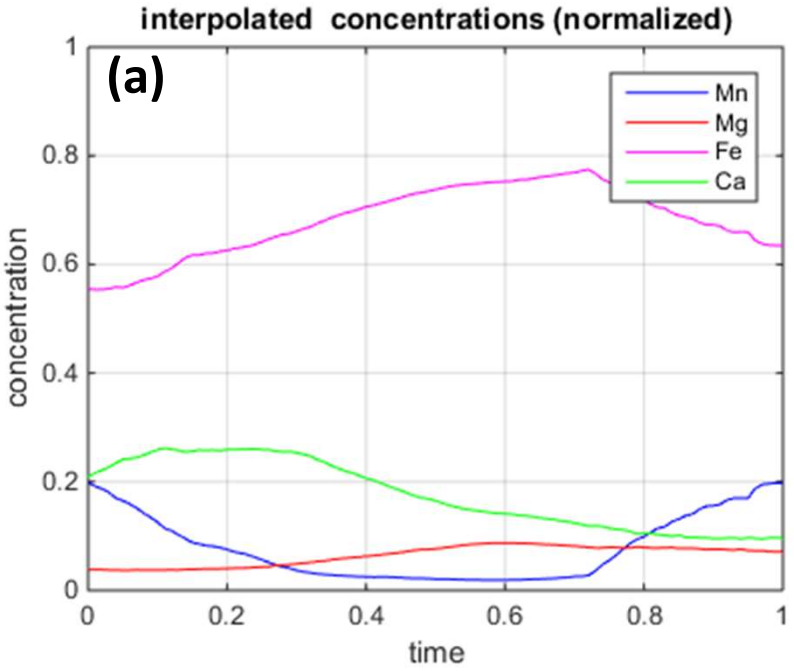
This will allow to see the increase of garnet volume content (GV) with time and temperature during prograde stage.

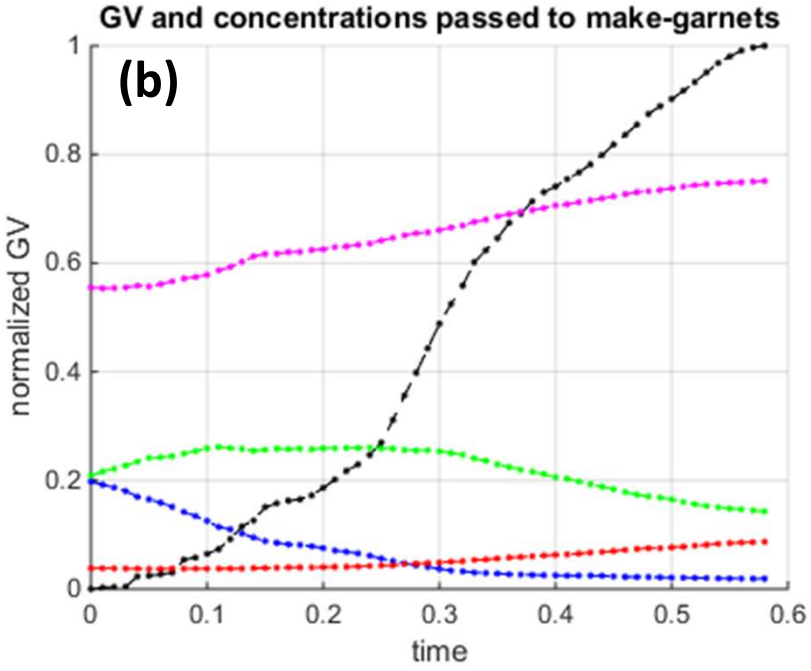






Concentration (Mn, Mg, Fe, Ca) and volume (GV) change (black dashed line) with time.
(a) based on the isopleth along the whole PT path
(b) only prograde stage

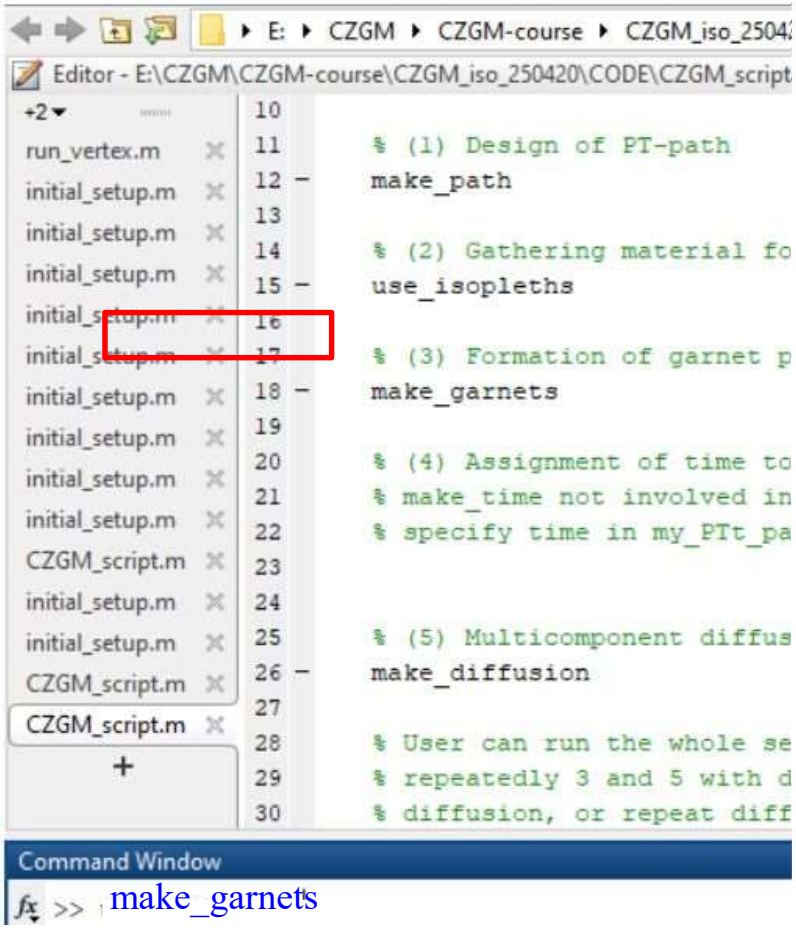


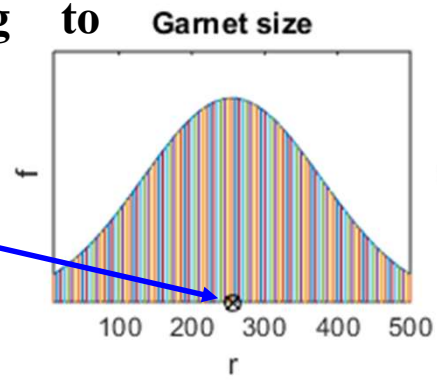


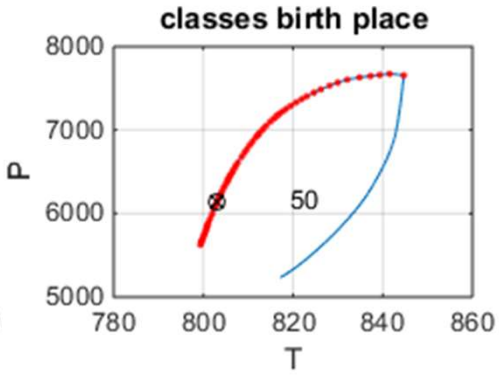
Step 3: make_garnets

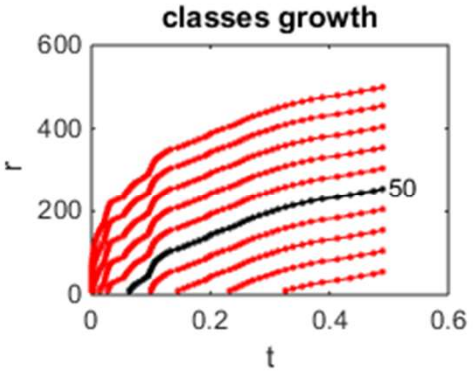
Population of garnets of predefined size distribution is generated according to previously computed GV.

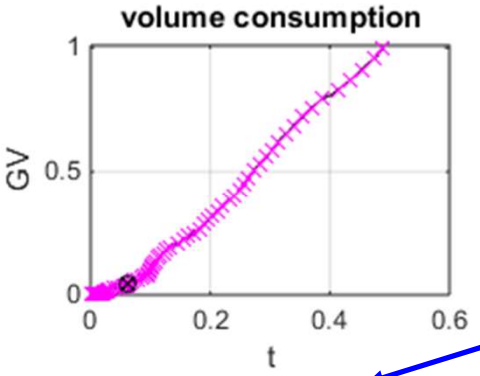
The selected garnet will undergo diffusion.

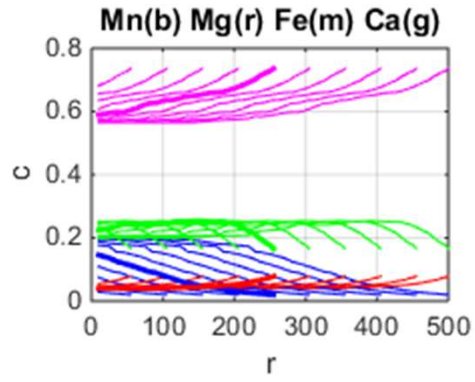












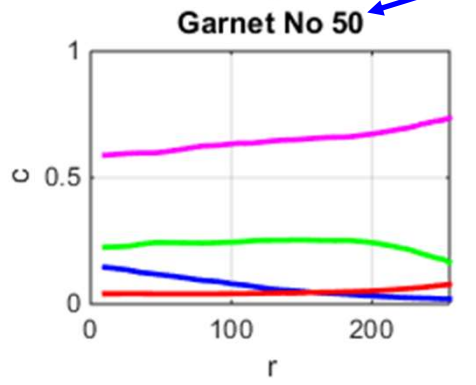
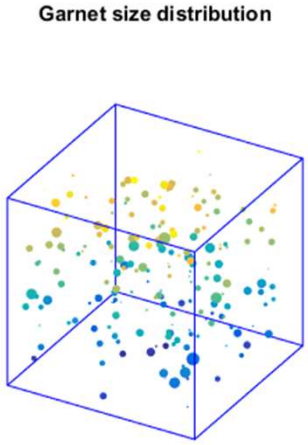
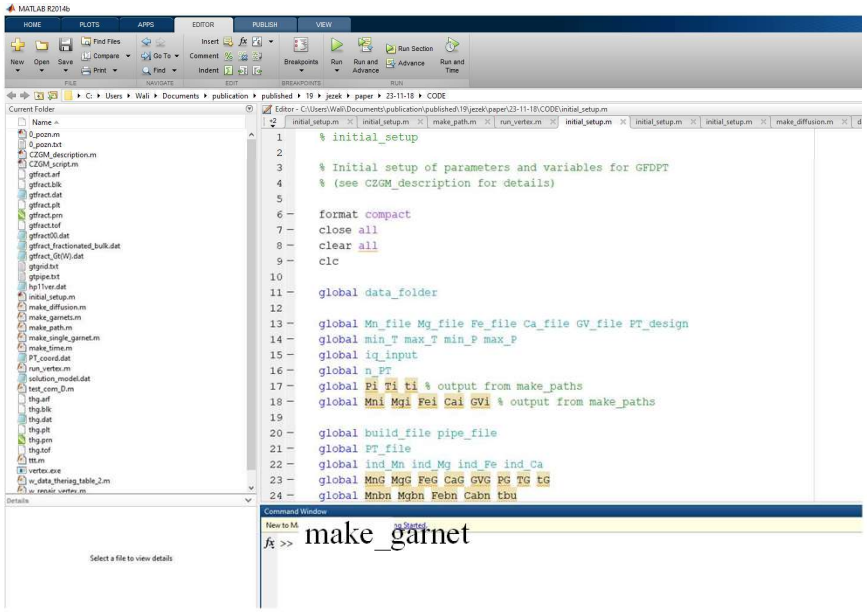
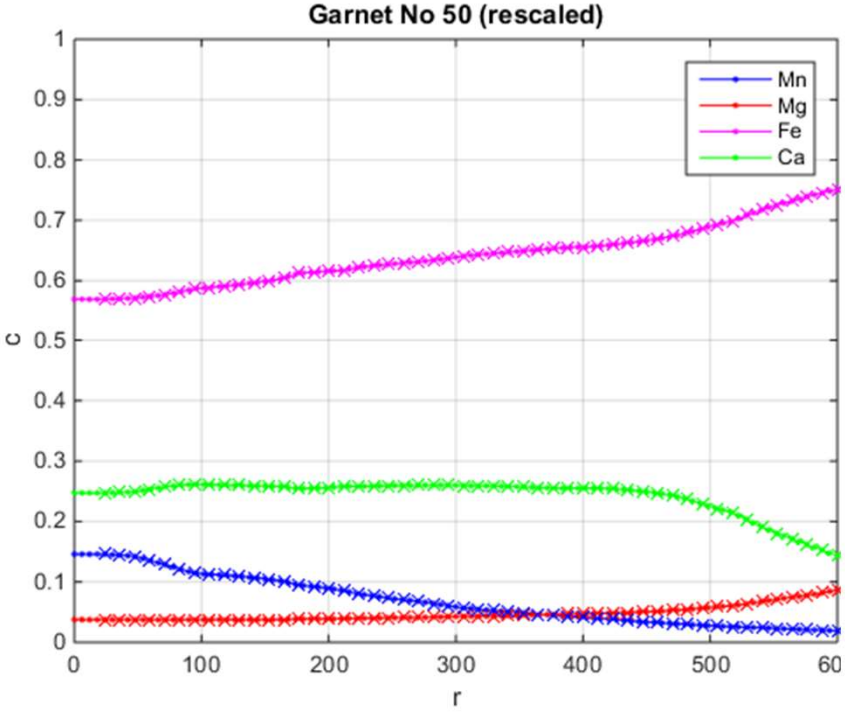
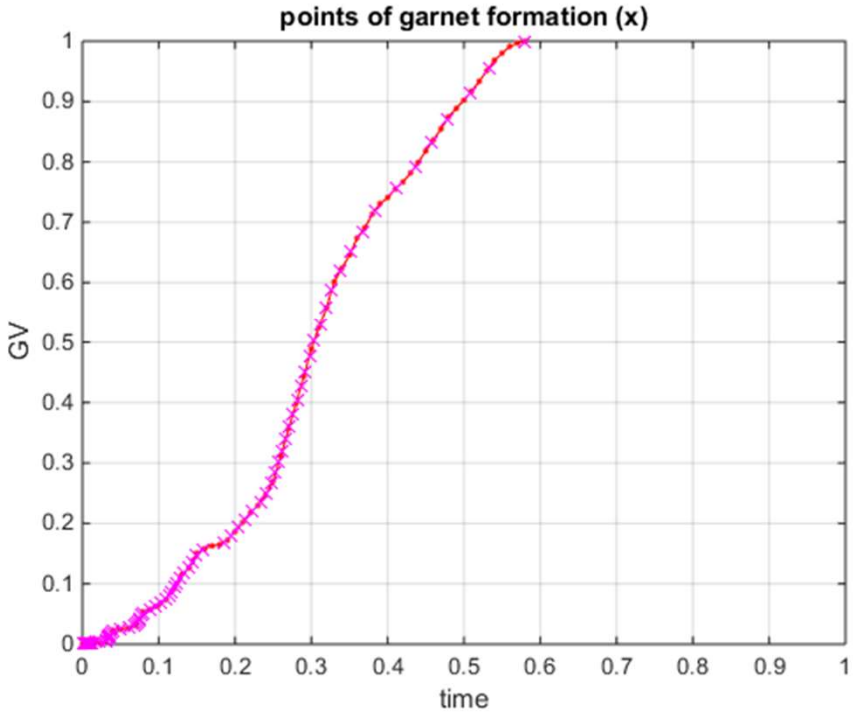


Illustration of initial profile and formation of garnet with time



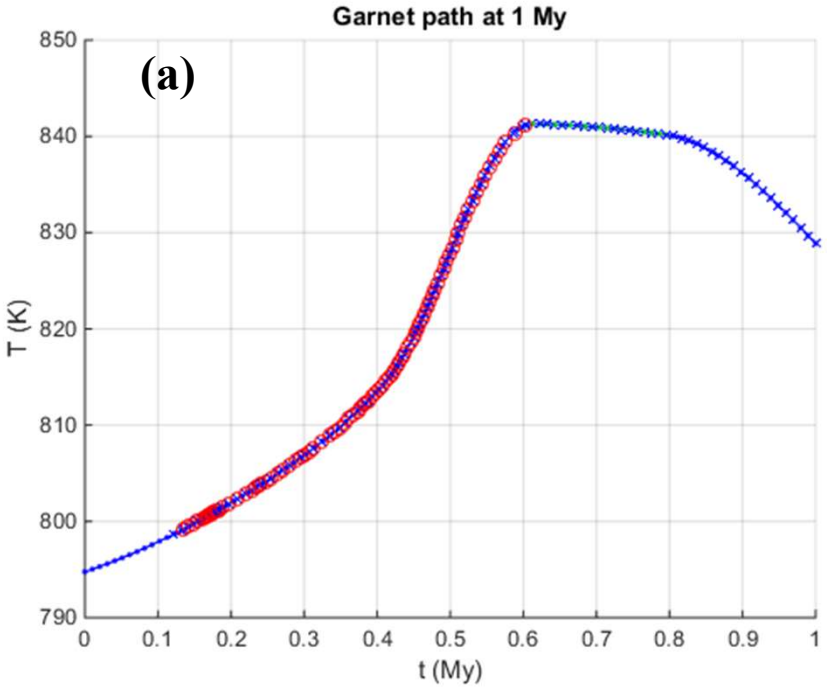




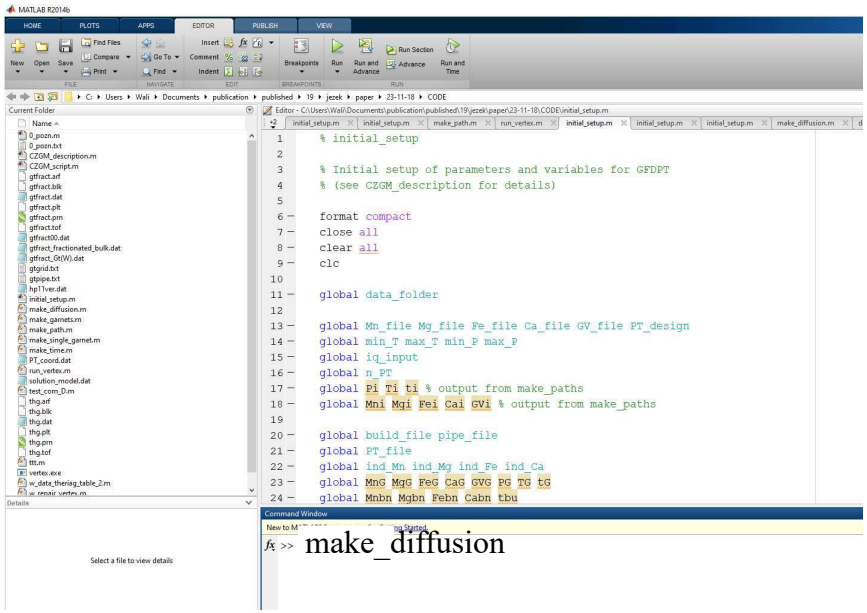


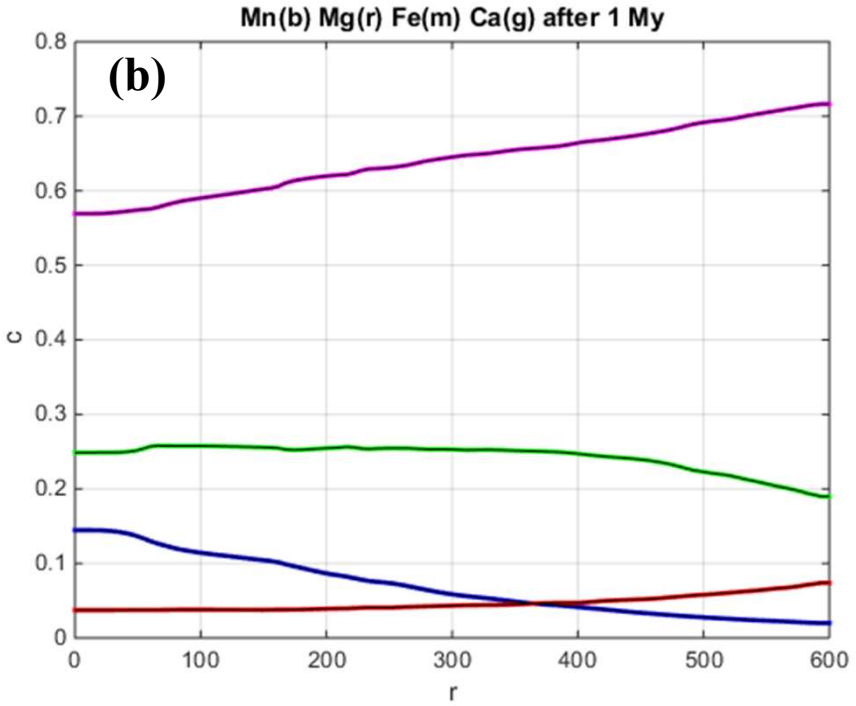
Step 4: make_diffusion

As the time scale is fixed to 1 Ma (Fig. a): “time_fac= 1”
and maximum temperatures reached are below 843 K (570 ºC), no diffusion occurs (Fig. b)



Diffusion of garnet no 50 after 1 Ma

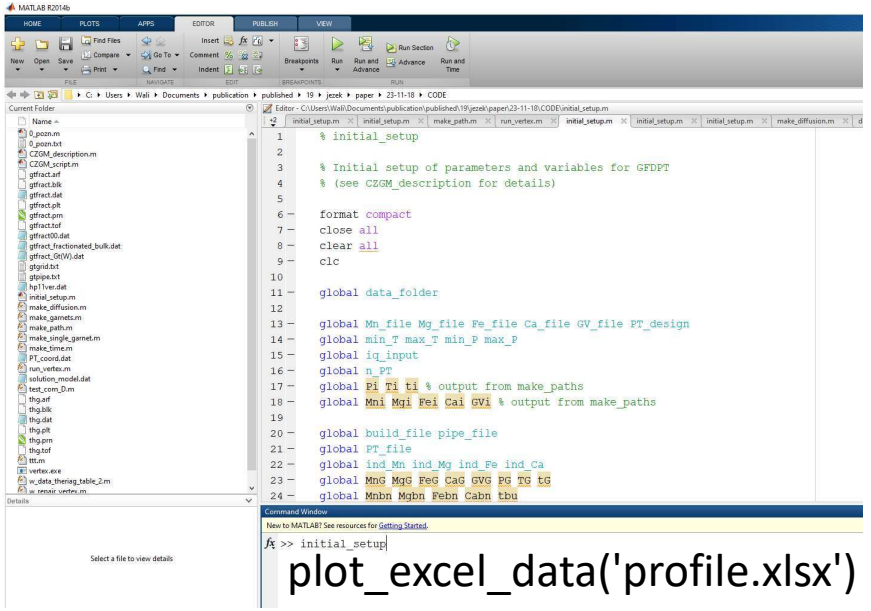


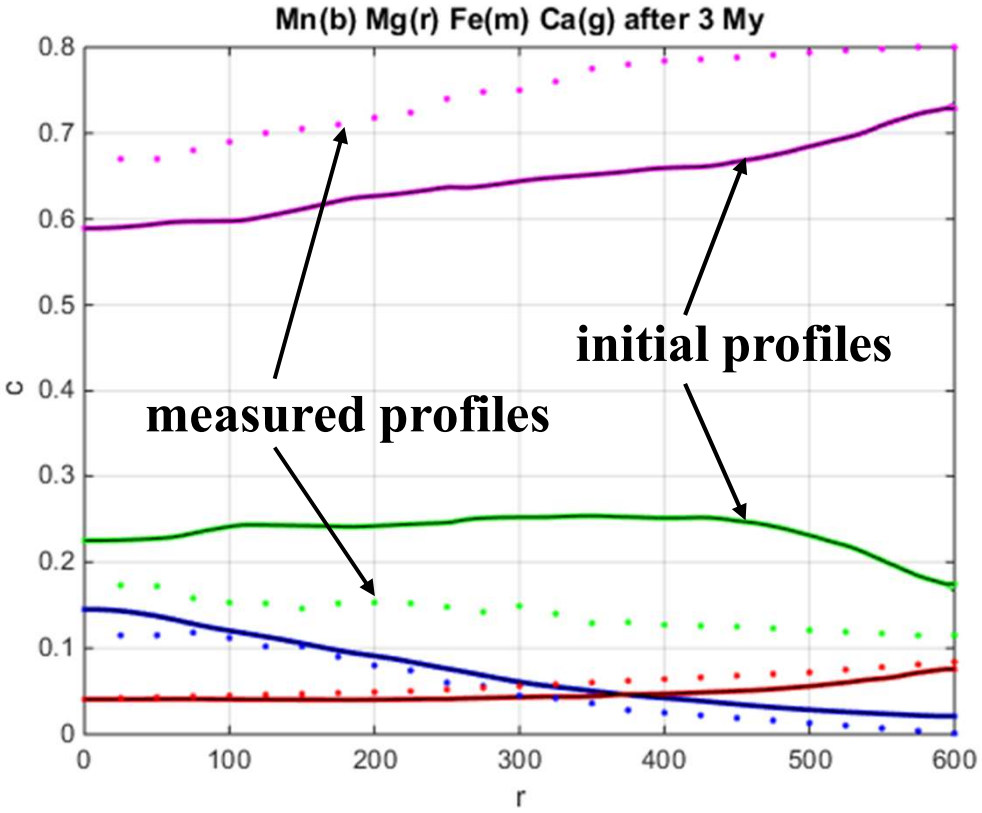


Post-processing:

Plotting of measured profiles

To compare the calculated profiles with that measured, call data from the measured profile in Excel:
plot_excel_data('profile.xlsx')

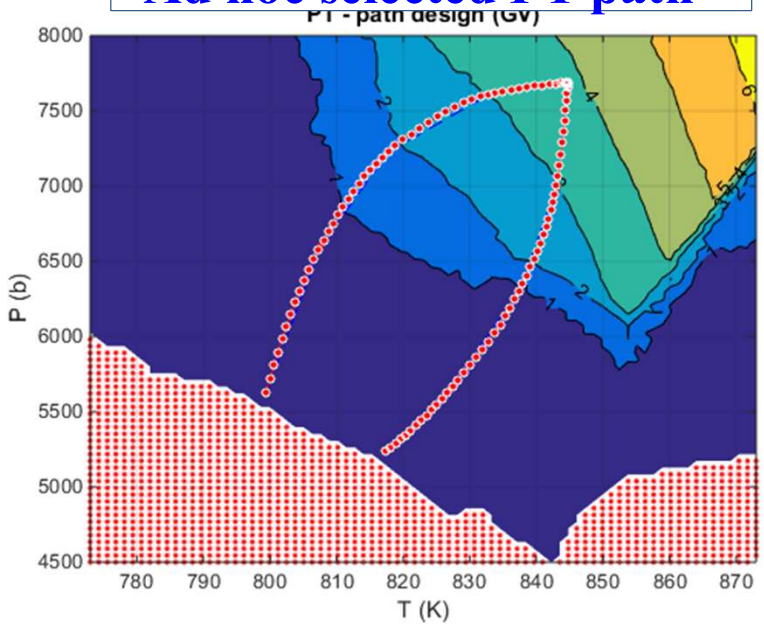




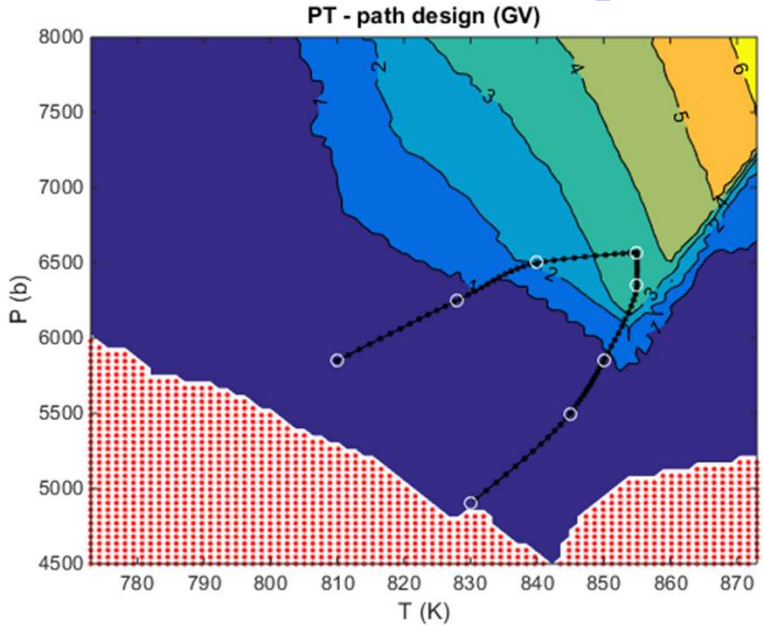
If the modelling was successful, the final (after diffusion) profiles should be close to the measured profiles (dashed lines). As there was no diffusion in the treated garnet, this means the PT path was not correctly selected. We will continue to try changing the PT path and possibly seect another garnets (garnet_no) to find the best agreement between model and experimental lines.

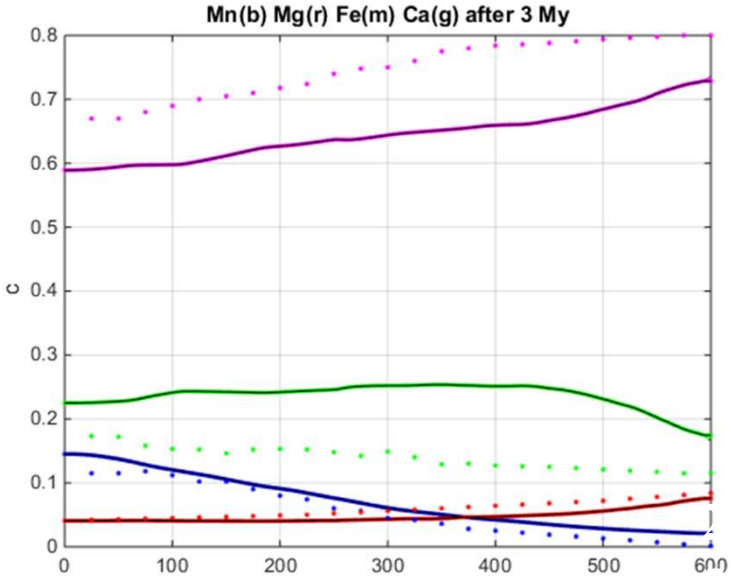
Examples from two ad hoc selected and corrected PT paths

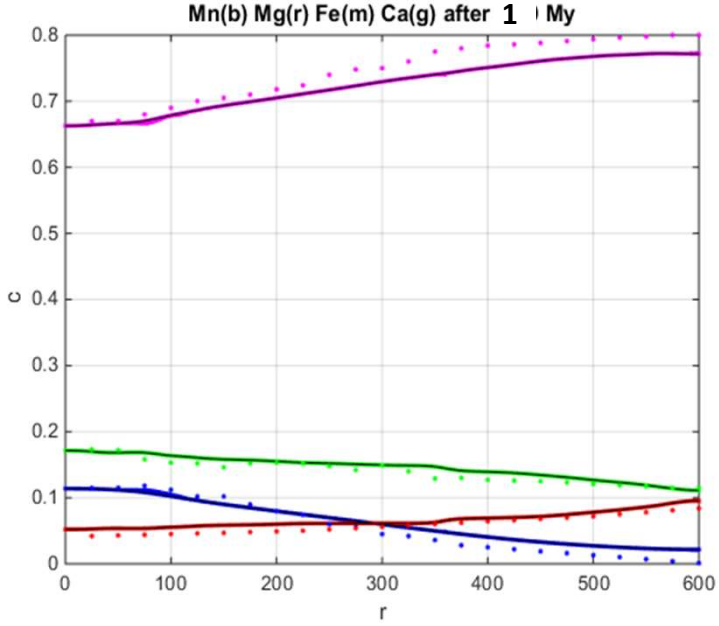
Ad hoc selected PT path



The corrected PT path

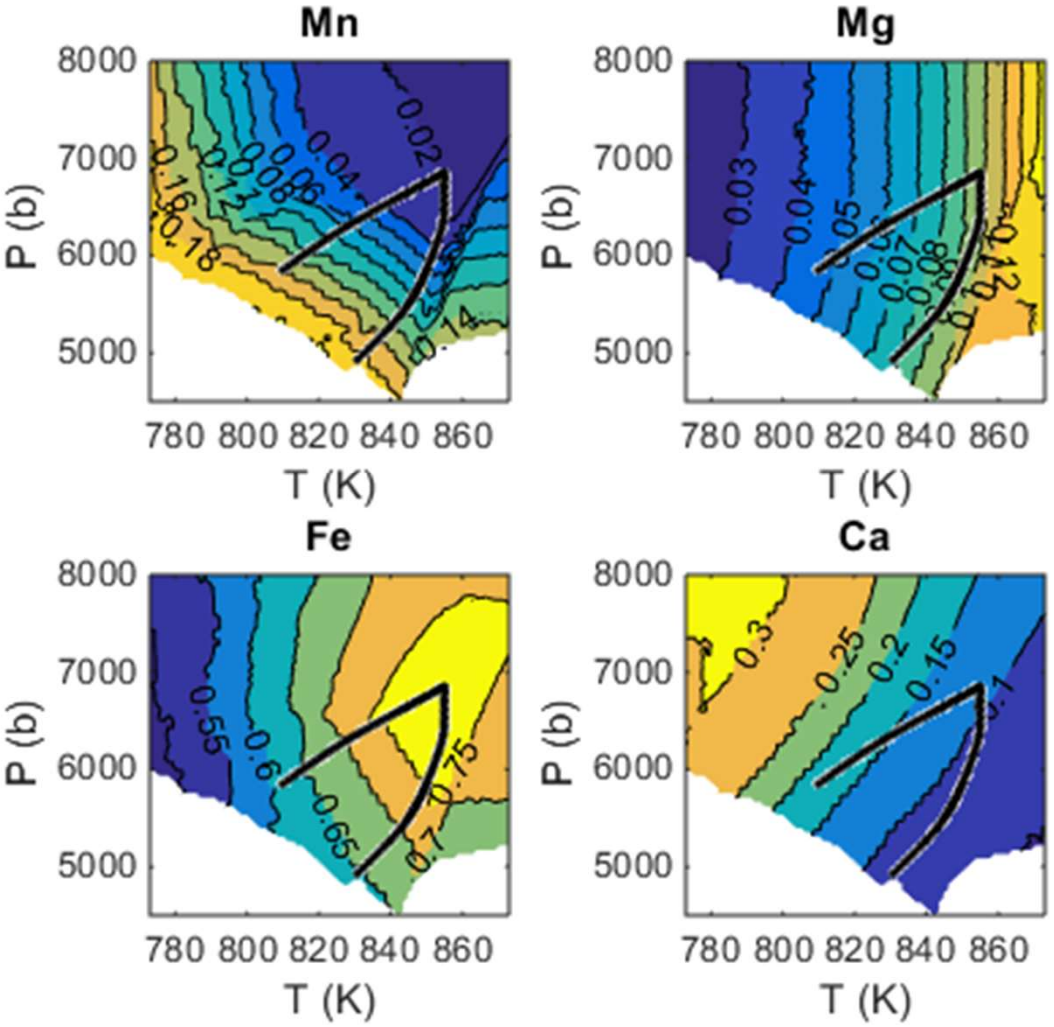


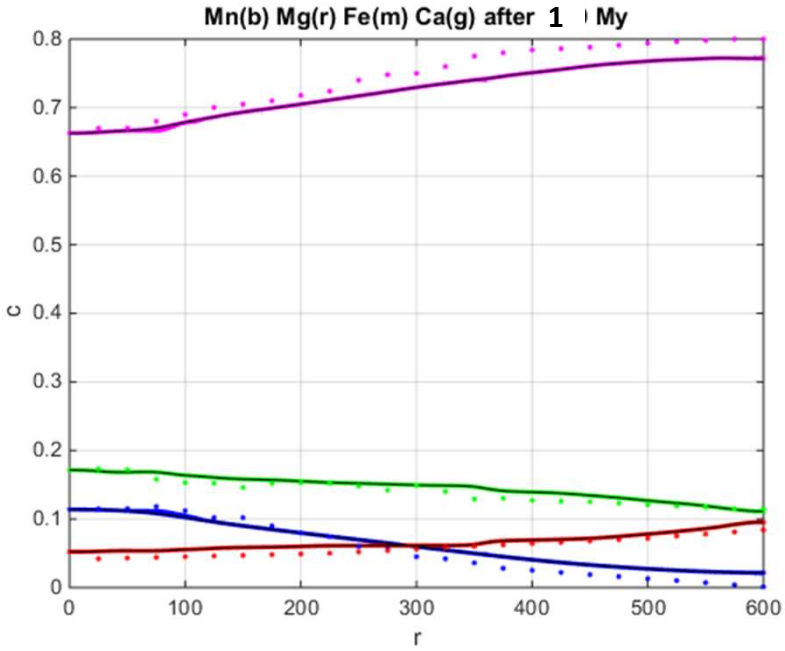




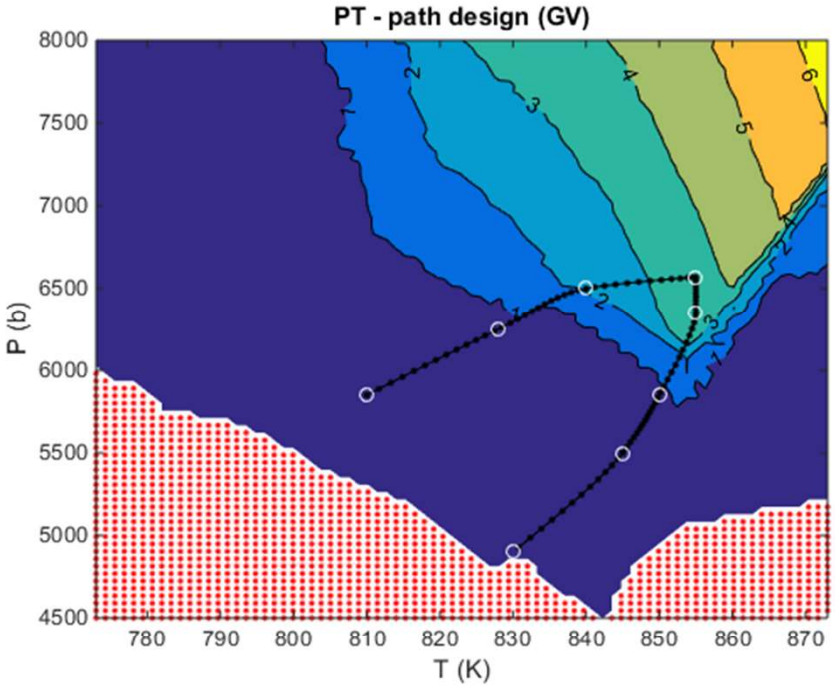
To reach a best agreement between initial and measured profile, it is needed to change the position of PT path based on compositional isopleths

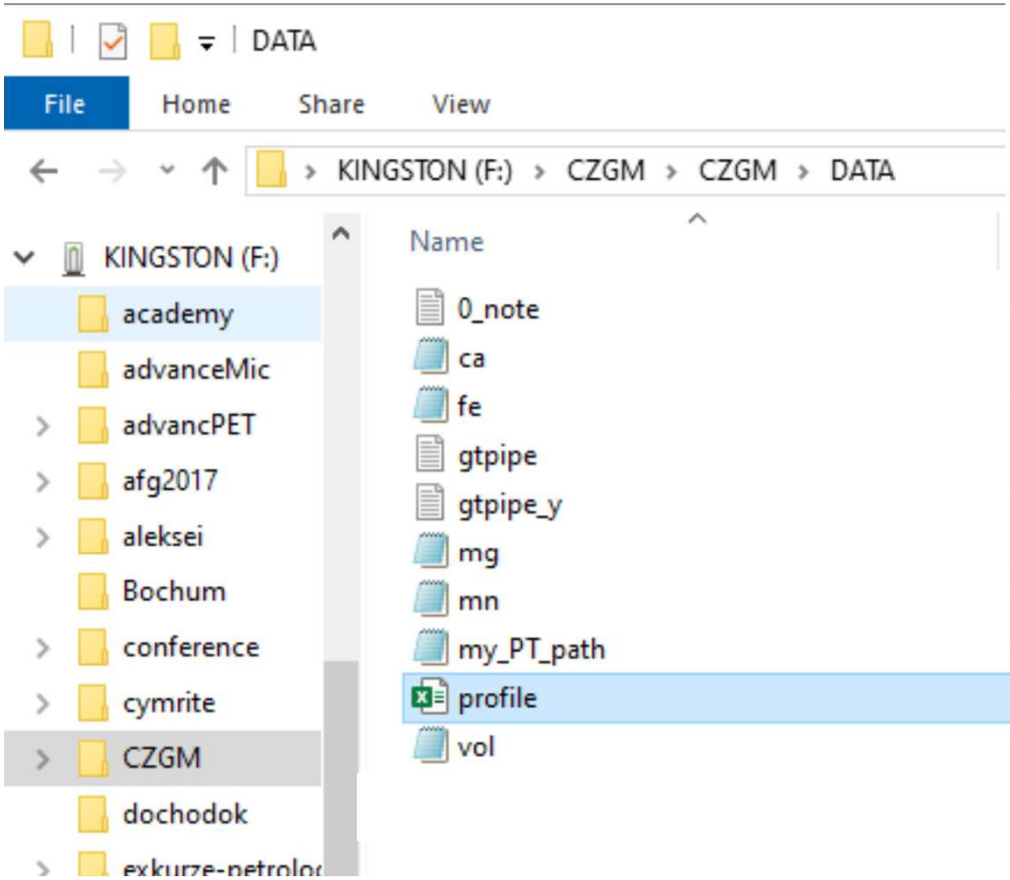
Variation of garnet_no can also help to adjust or get the best fit.





After finding the best fit, the PT values for the corresponding PT path can be added to the file my_PT_path.dat. The time duration for each PT sector along the PT path can be also defined in the created file my_PTt_path.dat.





P[bar]	T[K]	t
5850	810	0
6250	828	0.1
6500	840	0.2
6570	855	0.3
6350	855	1.0
5850	850	1.5
5500	845	1.6
4900	830	1.7

Parameters that can be changed from command line include:

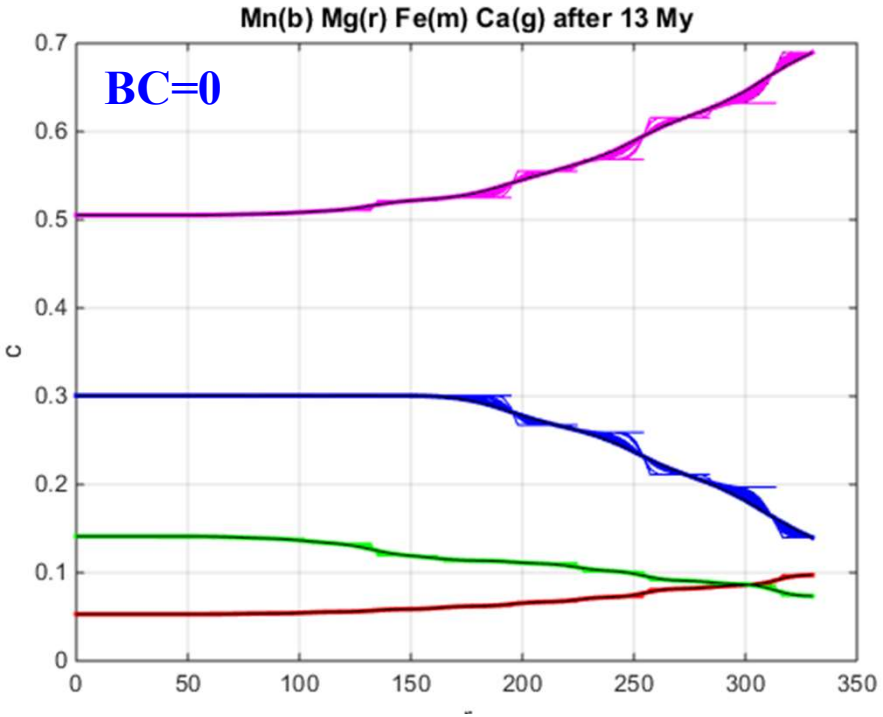
garnet_no=e.g. 25
This defines the position, where garnet started to grow along the selected PT path

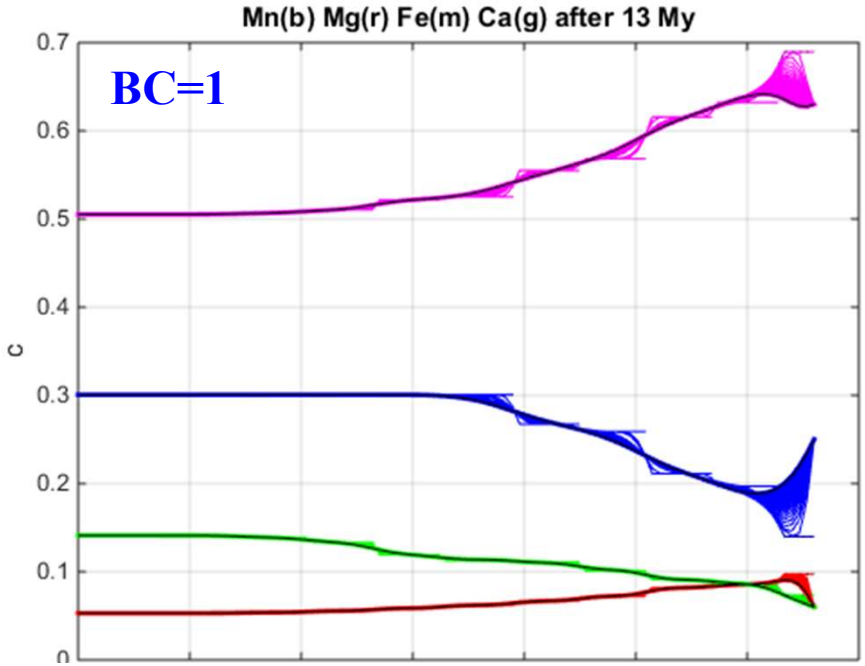
ime_fac=10
This factor multiplies actual time scale. If temperature is high, the time factor can substantially modify compositional zoning in garnet

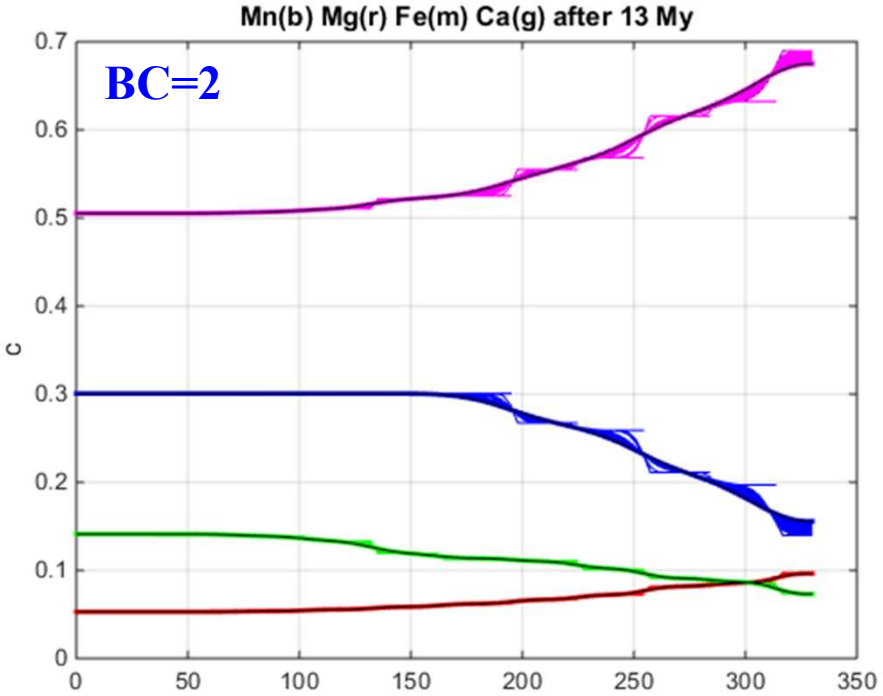
BC=3
In some cases the rim of already completed garnet can be modified during cooling (remaining path). In this case boundary conditions applied in diffusion should be changed appropriately.

Examples of boundary conditions for the remaining part of the PT-path:

BC=0: fixed boundary concentrations on the garnet rim
BC=1: concentrations defined by user
BC=2: closed system (zero gradient)
BC=3: Fe, Mg and Ca interpolated from the PT-grids (isopleths) while Mn=0

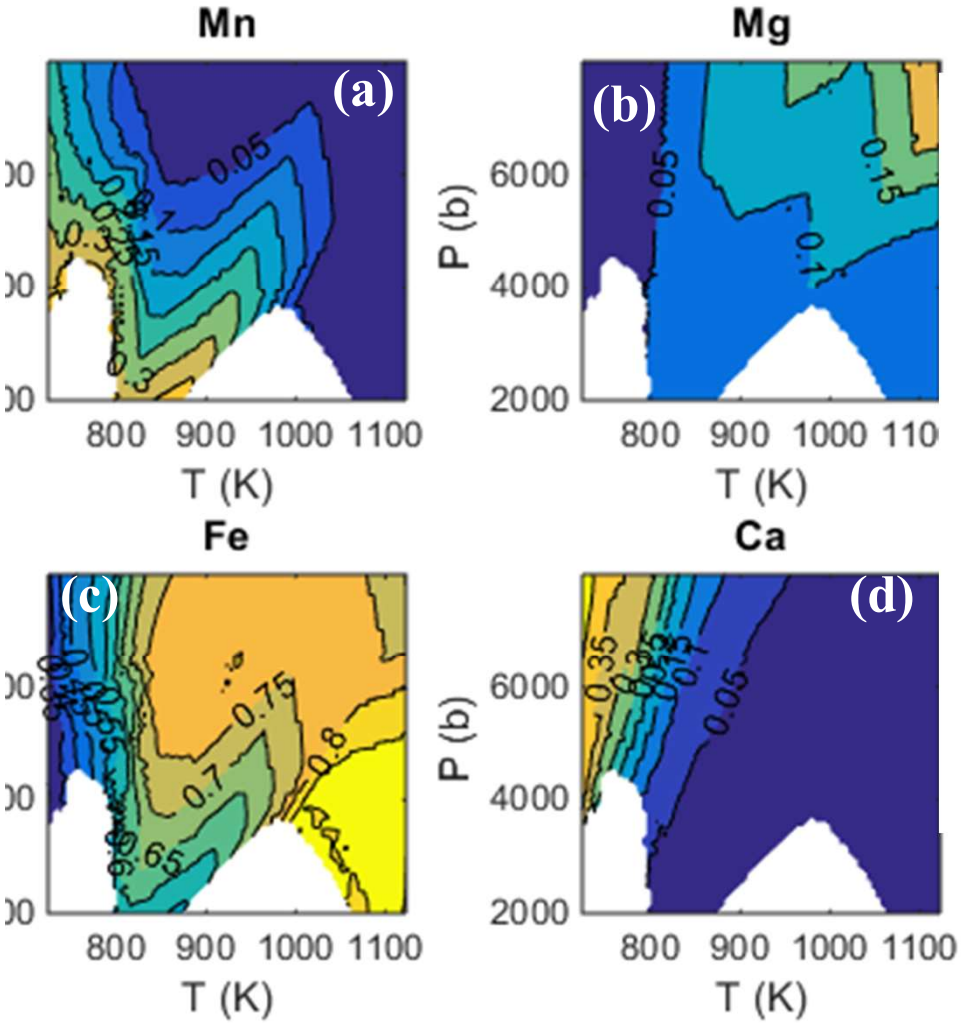


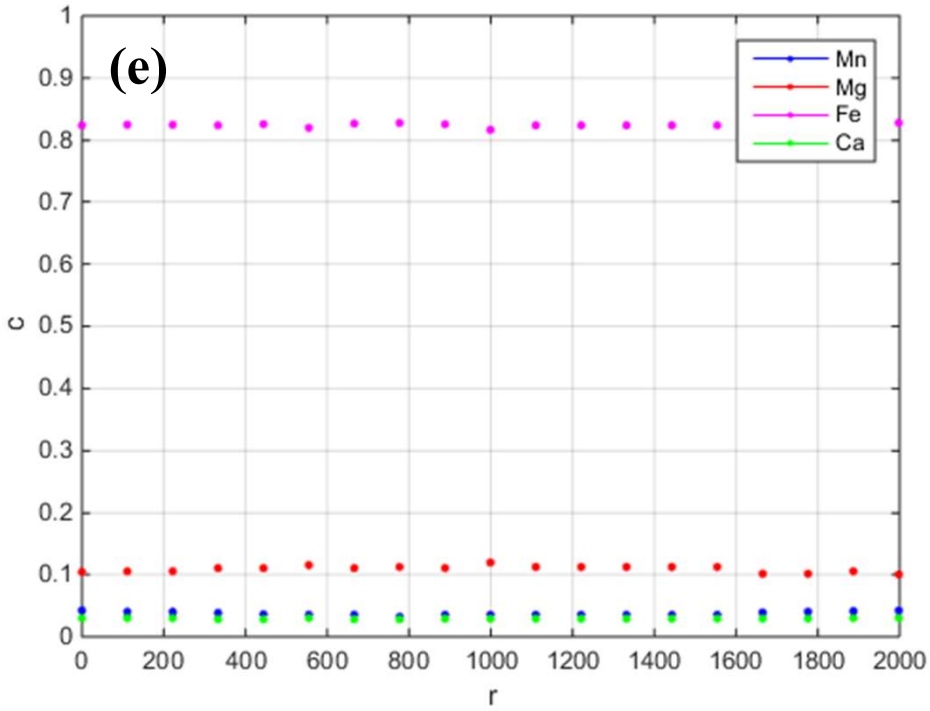




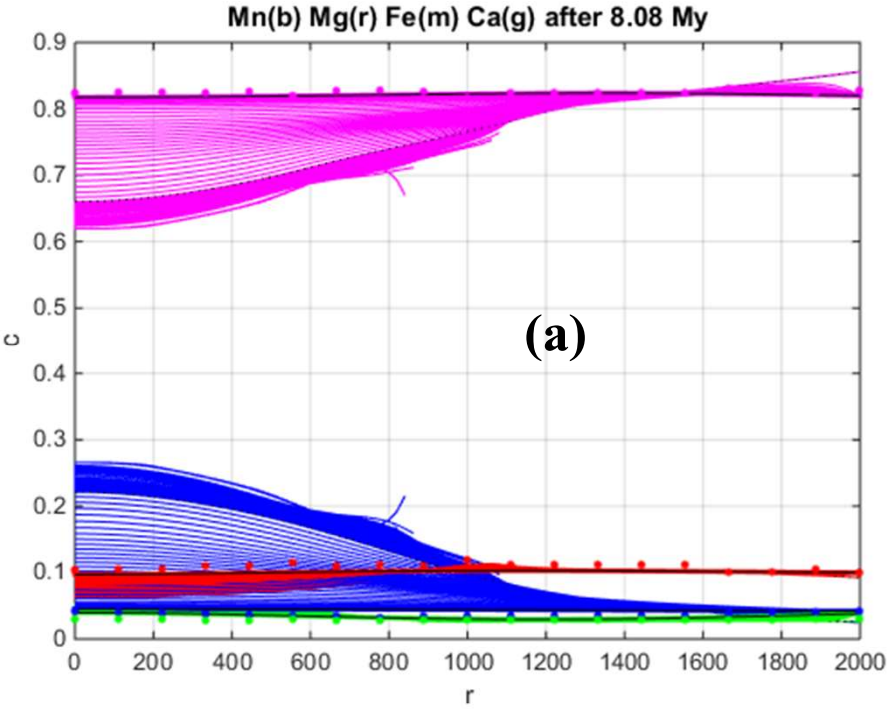
Example of almost homogenized garnet from high-grade terrane

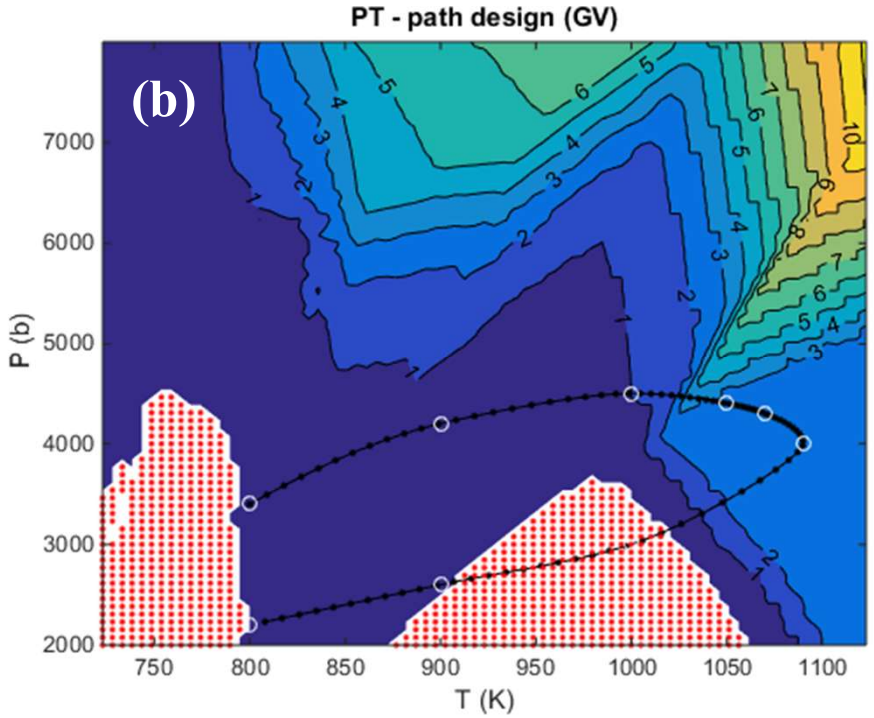
Compositional isopleths (a-d), measured compositional profiles (e) of garnet (2 mm in size)

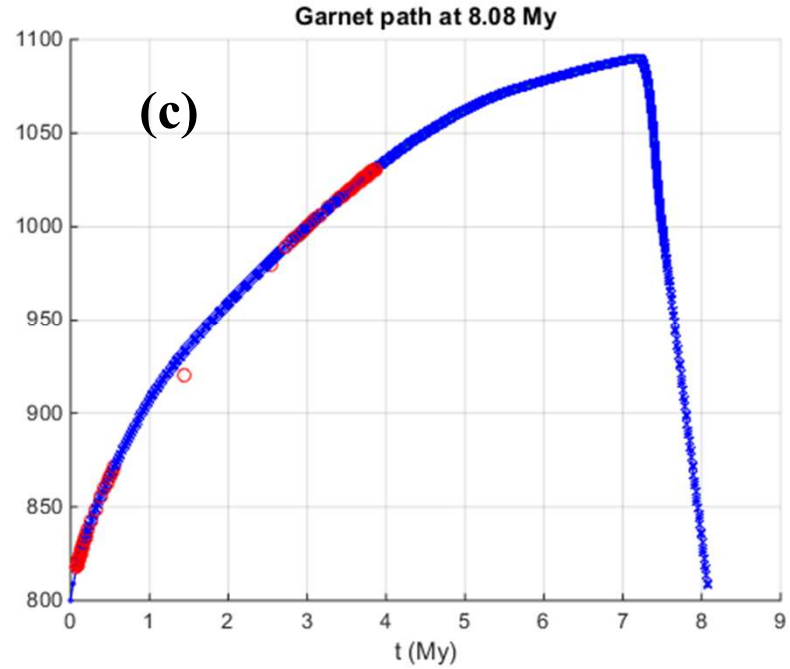




The best fits between measured (dotted) and simulated (lines) profiles (a), obtained for the PT path (b) and time duration (c)

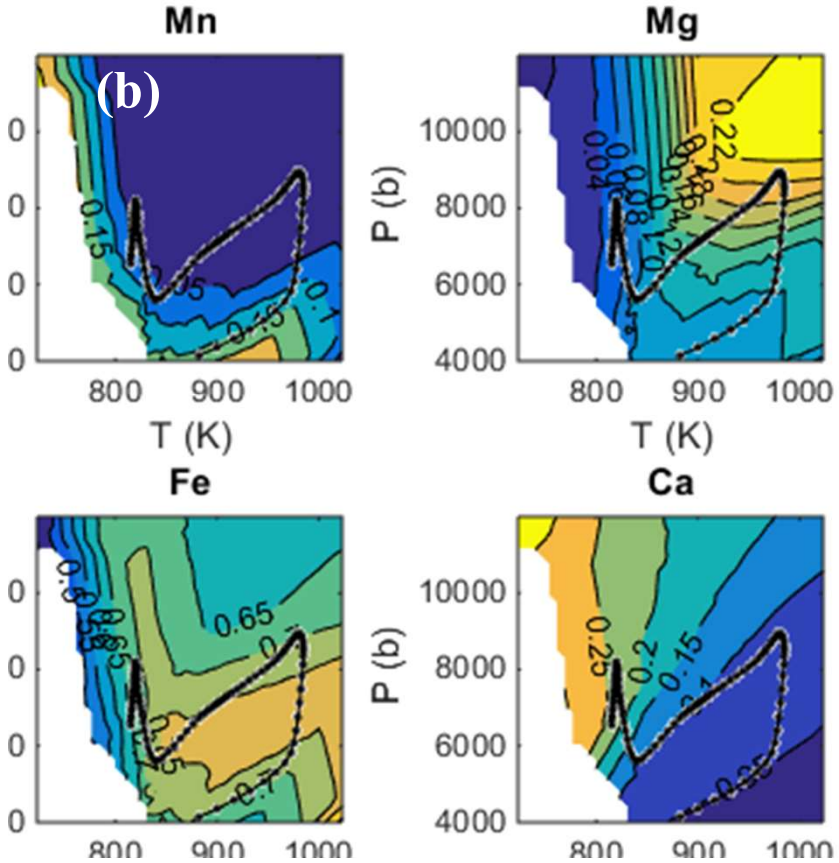


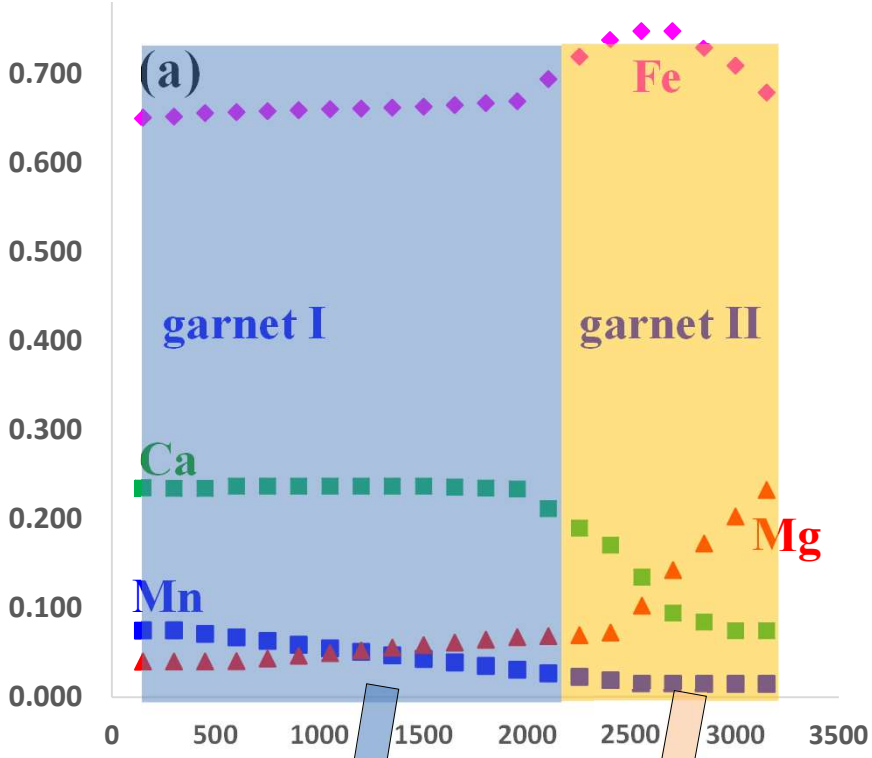


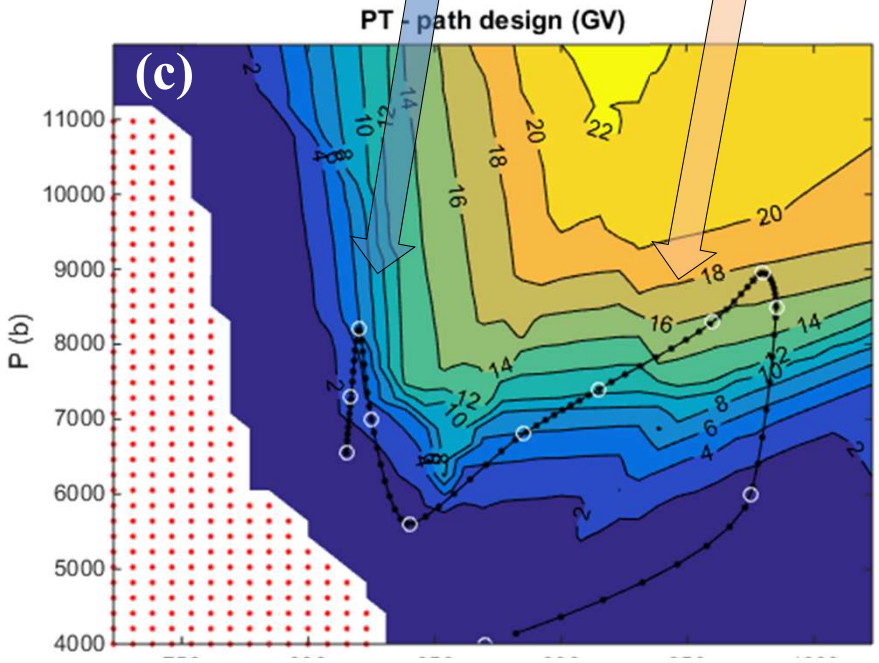


Examples of two or more garnet-growing events:

Here garnet shows two stage growing zoning (I and II). The core with high Ca content (a) formed at T<830 K (b, c) and rim with high Mg at higher T







The best fits are obtained for the selected PT path with an earlier accretionary and subsequent barrovian type metamorphism and time duration of 15 Ma as below