

CZGM-iso

The **CZGM** (**C**ompositional **Z**oning in **G**arnet and its **M**odification 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:

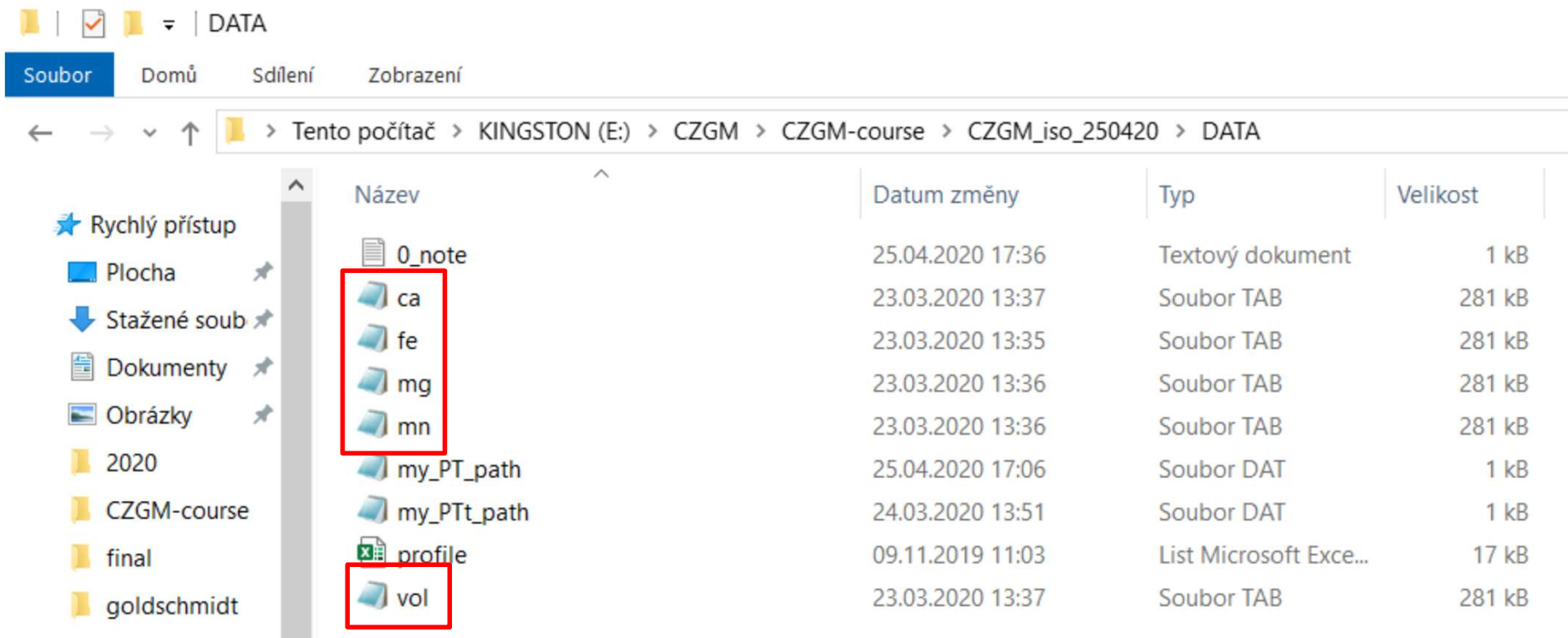
After calculation of pseudosection using Vertex (version 2019), compositional isopleths for garnet should be calculated using Werami.

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.

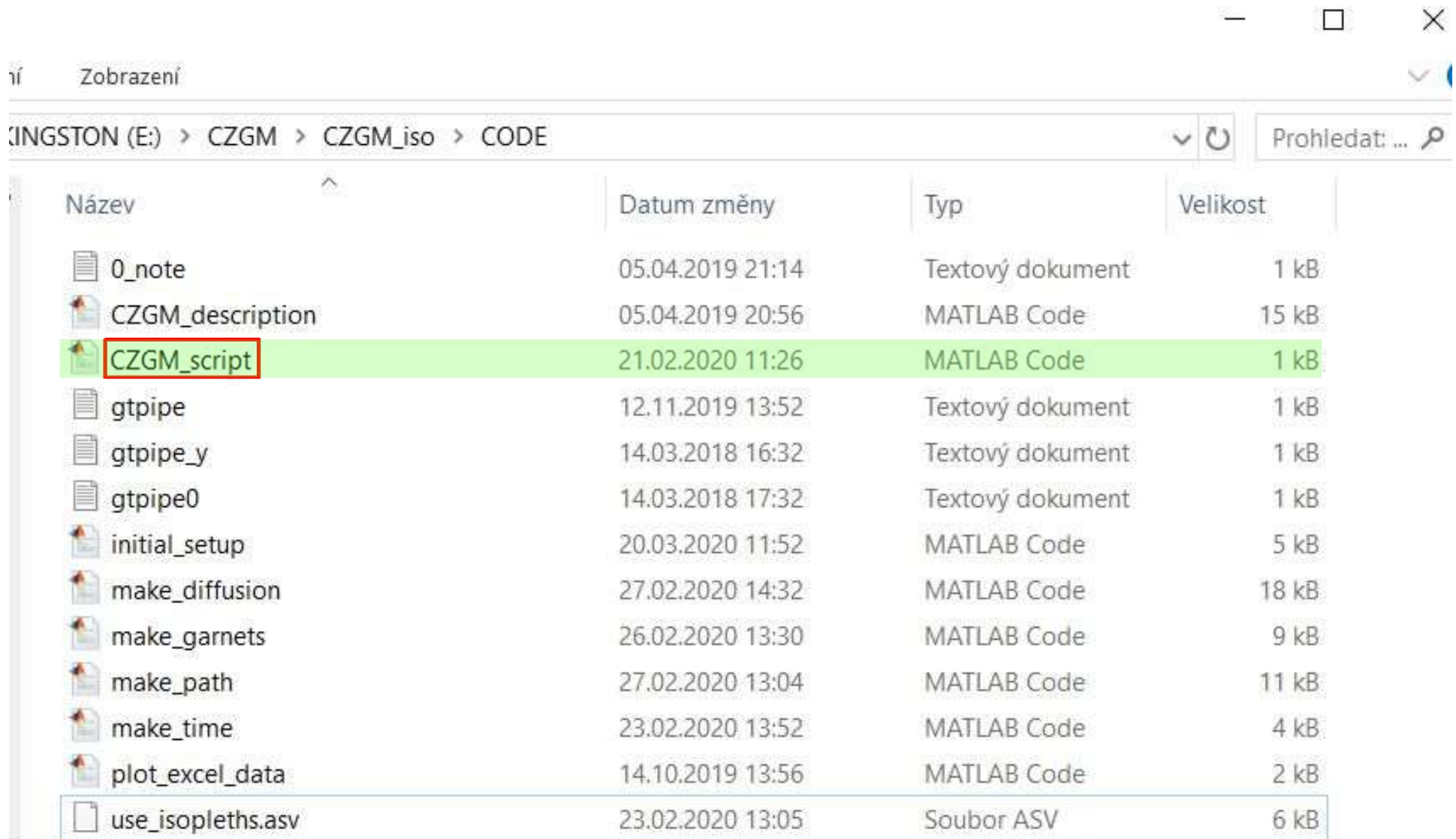
The screenshot shows a Windows File Explorer window with the address bar set to 'KINGSTON (F:) > CZGM > CZGM > DATA'. The left pane shows a list of folders including 'academy', 'advanceMic', 'advancPET', 'afg2017', 'aleksei', 'Bochum', 'conference', 'cymrite', 'CZGM', 'dochodok', and 'exkurze-petrolog'. The right pane shows a list of files: '0_note', 'ca', 'fe', 'gtpipe', 'gtpipe_y', 'mg', 'mn', 'my_PT_path', 'profile', 'vol', and 'gtfract'. The 'profile' file is highlighted with a red box.

Overlaid on the right side of the File Explorer is an Excel spreadsheet. The spreadsheet has a green header bar with 'Automatické ukládání' and a ribbon with 'Soubor', 'Domů', 'Vložení', 'Rozložení stránky', and 'Vzorci'. The active cell is H10. The spreadsheet contains the following data:

	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 initial_setup

MATLAB R2014b

HOME PLOTS APPS EDITOR PUBLISH VIEW

E:\CZGM\CZGM_iso\CODE

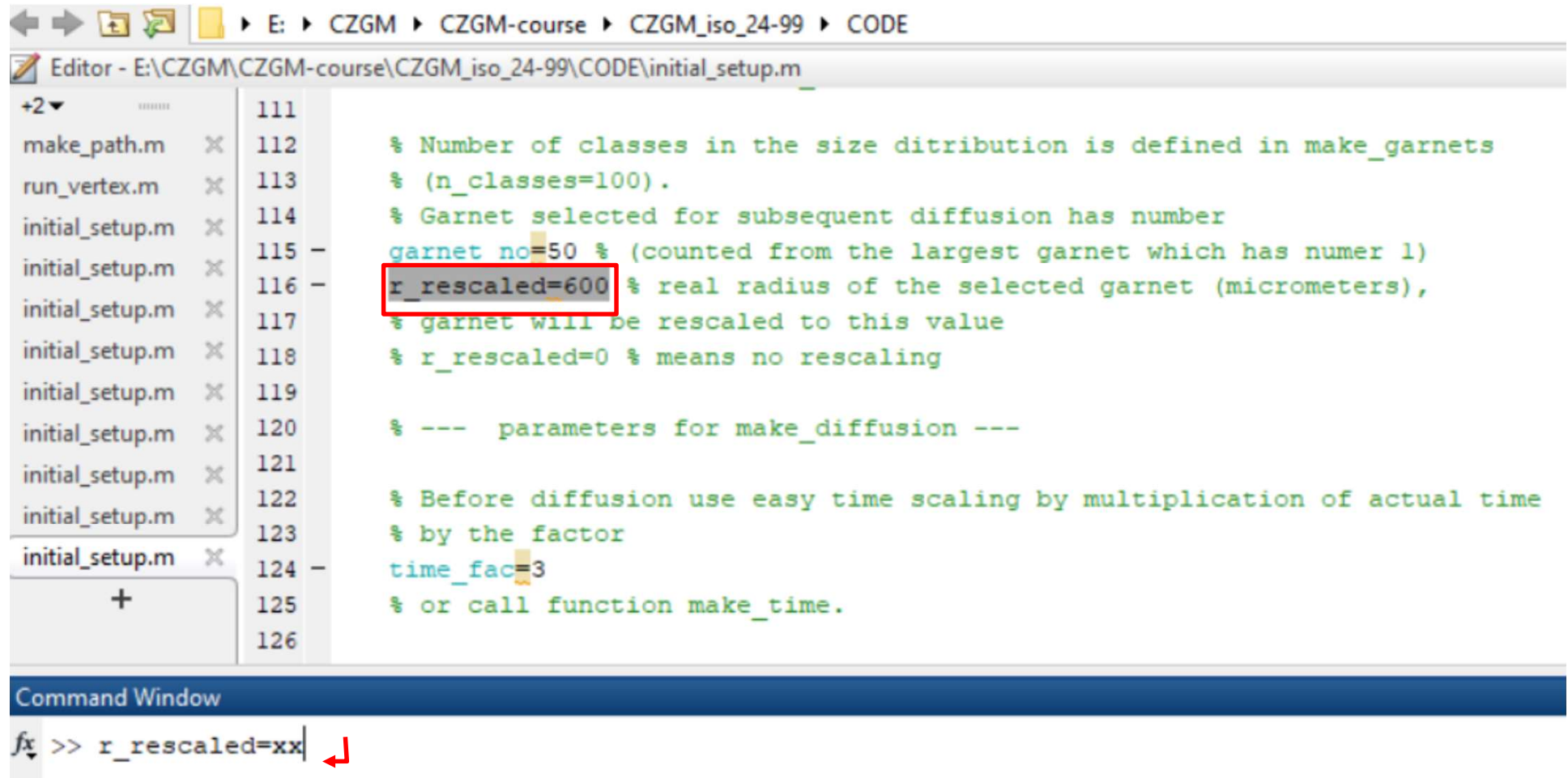
Editor - E:\CZGM\CZGM_iso\CODE\initial_setup.m

```
1
2 % initial_setup
3 % Initial setup of parameters and variables for CZGM
4 % (see CZGM_description for details)
5
6 - format compact
7 - close all
8 - clear all
9 - clc
10
11 - global data_folder
12
13 - global Mn_file Mg_file Fe_file Ca_file GV_file PT_design
14 - global min_T max_T min_P max_P
15 - global iq_input
16 - global n_PT_pts
17 - global Pi Ti ti % output from make_paths
18 - global Mni Mgi Fei Cai GVi % output from make_paths
19
20 - global build_file pipe_file
21 - global PT_file
22 - global ind_Mn ind_Mg ind_Fe ind_Ca
23 - global MnG MgG FeG CaG GVG PG TG tG
24 - global Mbn Mgbn Febn Cabn tbu
25 - global iq_int
26
```

Command Window

```
600
time_fac =
    3
diff_mode =
    1
BC =
    2
B_conc =
    0.0400    0.1250    0.7780    0.0570
iq_JJ =
    0
fx >> initial_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)

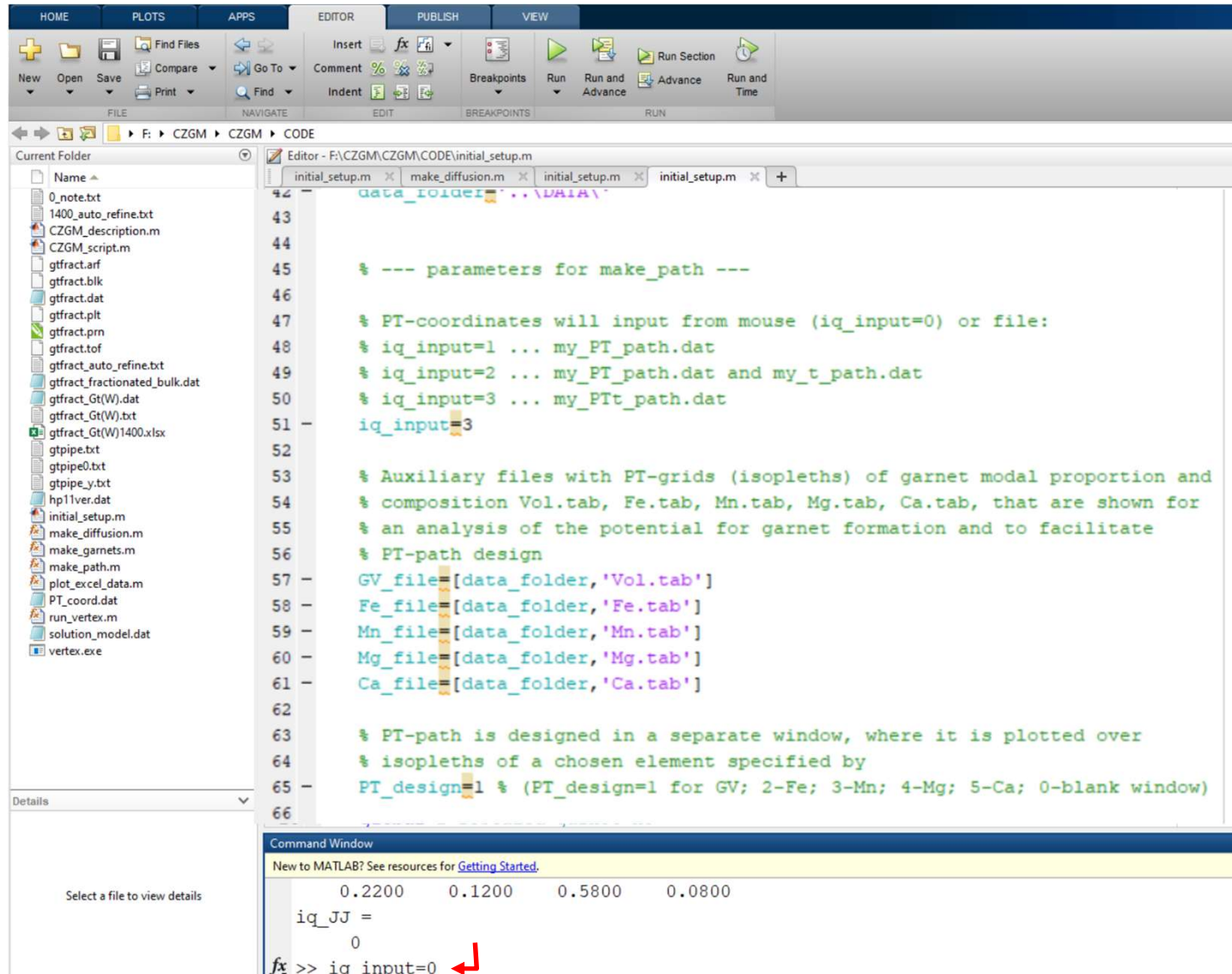


```
E:\CZGM\CZGM-course\CZGM_iso_24-99\CODE
Editor - E:\CZGM\CZGM-course\CZGM_iso_24-99\CODE\initial_setup.m
+2 111
make_path.m x 112 % Number of classes in the size ditribution is defined in make_garnets
run_vertex.m x 113 % (n_classes=100).
initial_setup.m x 114 % Garnet selected for subsequent diffusion has number
initial_setup.m x 115 - garnet no=50 % (counted from the largest garnet which has numer 1)
initial_setup.m x 116 - r_rescaled=600 % real radius of the selected garnet (micrometers),
initial_setup.m x 117 % garnet will be rescaled to this value
initial_setup.m x 118 % r_rescaled=0 % means no rescaling
initial_setup.m x 119
initial_setup.m x 120 % --- parameters for make_diffusion ---
initial_setup.m x 121
initial_setup.m x 122 % Before diffusion use easy time scaling by multiplication of actual time
initial_setup.m x 123 % by the factor
initial_setup.m x 124 - time_fac=3
+ 125 % or call function make_time.
126

Command Window
fx >> r_rescaled=xx
```

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 screenshot displays the MATLAB Editor interface. The main window shows the script `initial_setup.m` with the following code:

```
42 data_folder = '\DATA\  
43  
44  
45 % --- parameters for make_path ---  
46  
47 % PT-coordinates will input from mouse (iq_input=0) or file:  
48 % iq_input=1 ... my_PT_path.dat  
49 % iq_input=2 ... my_PT_path.dat and my_t_path.dat  
50 % iq_input=3 ... my_PTt_path.dat  
51 iq_input=3  
52  
53 % Auxiliary files with PT-grids (isopleths) of garnet modal proportion and  
54 % composition Vol.tab, Fe.tab, Mn.tab, Mg.tab, Ca.tab, that are shown for  
55 % an analysis of the potential for garnet formation and to facilitate  
56 % PT-path design  
57 GV_file=[data_folder, 'Vol.tab']  
58 Fe_file=[data_folder, 'Fe.tab']  
59 Mn_file=[data_folder, 'Mn.tab']  
60 Mg_file=[data_folder, 'Mg.tab']  
61 Ca_file=[data_folder, 'Ca.tab']  
62  
63 % PT-path is designed in a separate window, where it is plotted over  
64 % isopleths of a chosen element specified by  
65 PT_design=1 % (PT_design=1 for GV; 2-Fe; 3-Mn; 4-Mg; 5-Ca; 0-blank window)  
66
```

The Command Window at the bottom shows the following output:

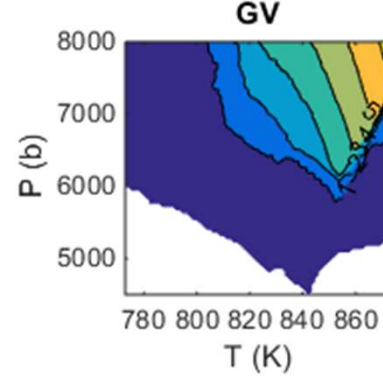
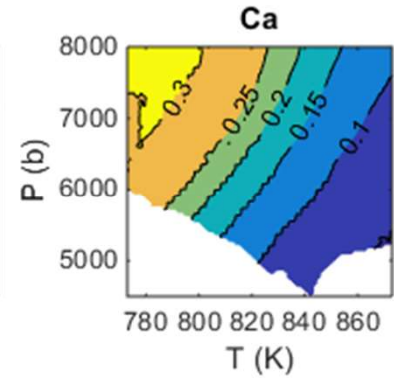
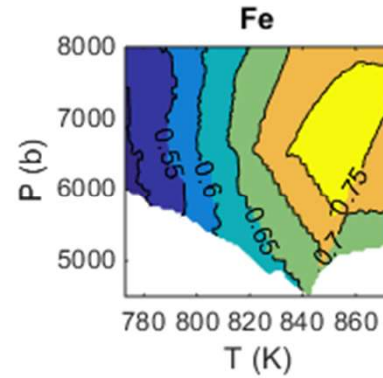
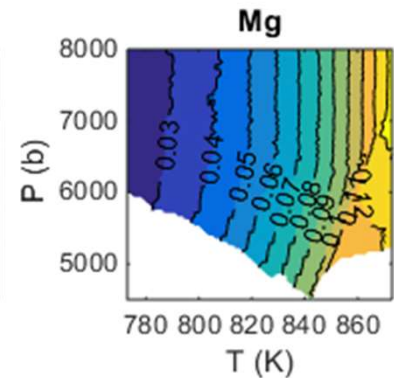
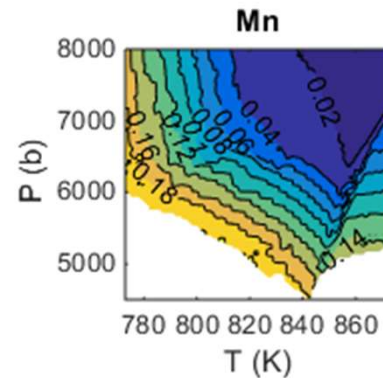
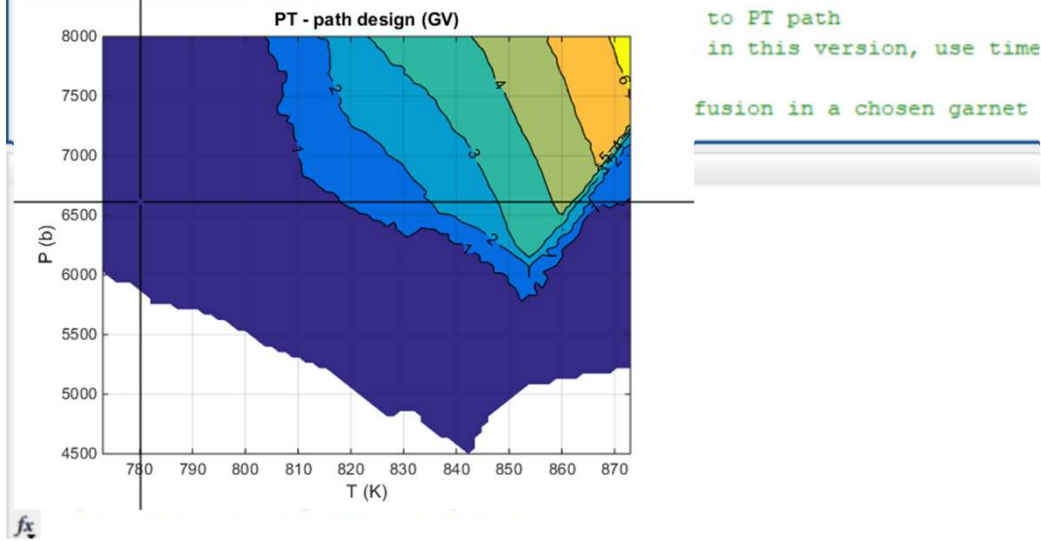
```
New to MATLAB? See resources for Getting Started.  
0.2200 0.1200 0.5800 0.0800  
iq_JJ =  
0  
fx >> iq_input=0
```

A red arrow points to the `iq_input=0` command in the Command Window.

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

```

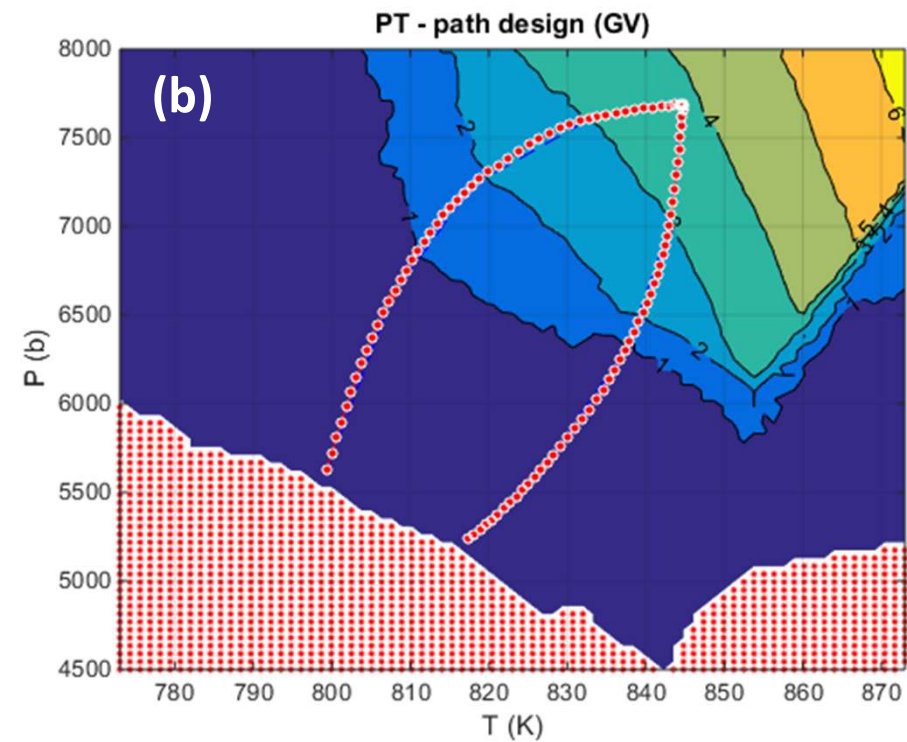
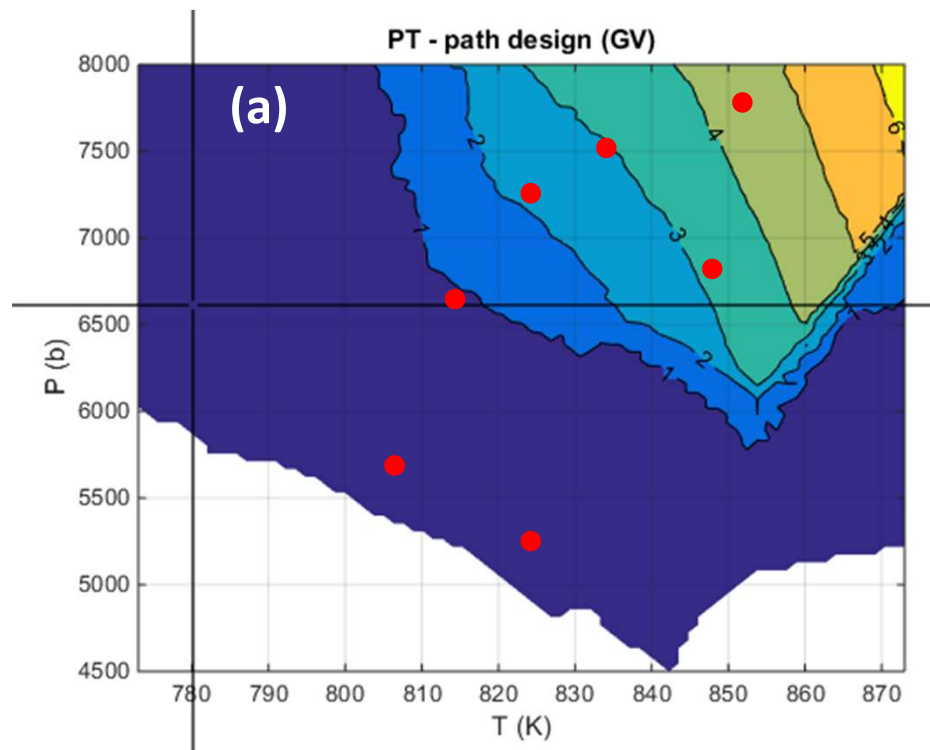
Editor - E:\CZGM\CZGM_iso_24-99\CODE\CZGM_script.m
-----
CZGM_description.m  X  1      % CZGM_script
initial_setup.m    X  2
initial_setup.m    X  3      % Compositional Zoning in Garnet and its Modificat
initial_setup.m    X  4
make_path.m        X  5      % Modelling with CZGM consists of the following st
run_setup.m        X  6      % (see the functions CZGM_description and initial_
initial_setup.m    X  7
initial_setup.m    X  8      % (0) Preparation and initial setup
CZGM_script.m      X  9      initial_setup
initial_setup.m    X 10
initial_setup.m    X 11      % (1) Design of PT-path
initial_setup.m    X 12      make_path
initial_setup.m    X 13
initial_setup.m    X 14      % (2) Gathering material for garnets
initial_setup.m    X 15      run_vertex % Fractionation along PT path
initial_setup.m    X 16      % or
initial_setup.m    X 17      use_isopleths % Interpolation from isopleths
initial_setup.m    X 18
initial_setup.m    X 19      % (3) Formation of garnet population
initial_setup.m    X 20      make_garnets
CZGM_script.m      X 21
  
```



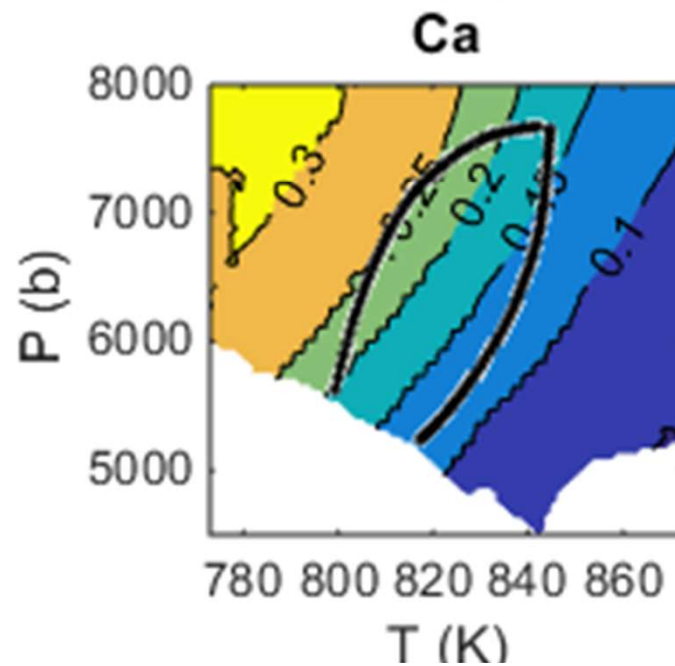
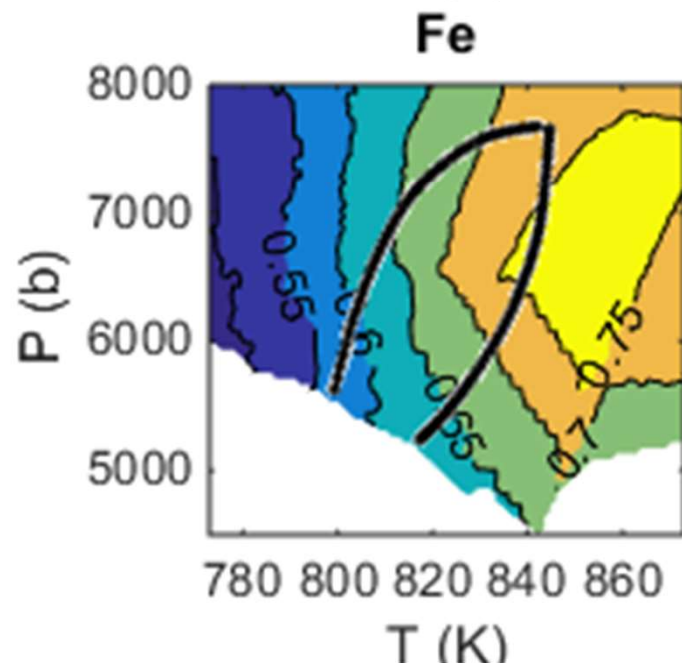
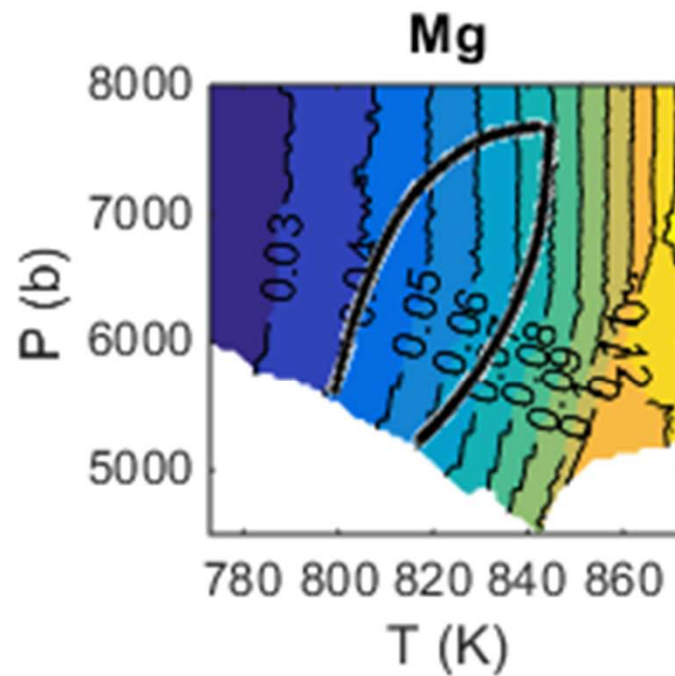
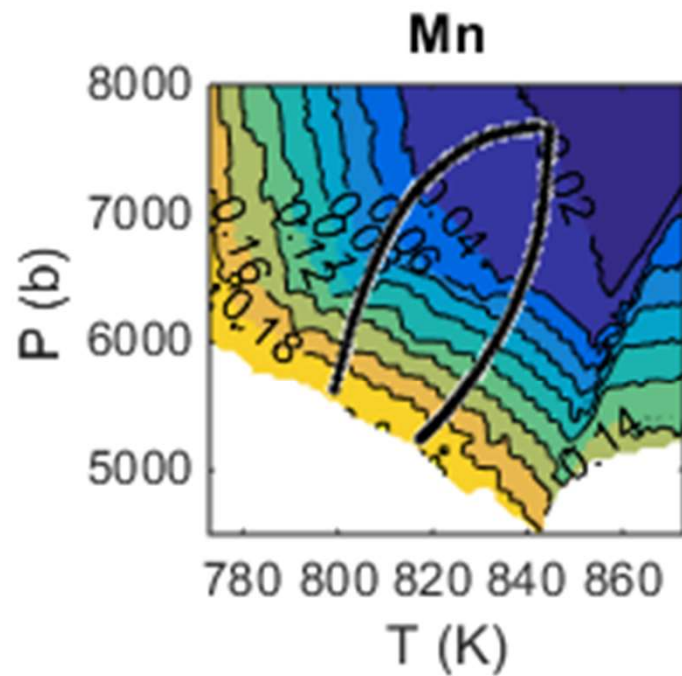
Constraining PT path by hand:

The image of garnet volume content (GV) is selected to draw the PT path.

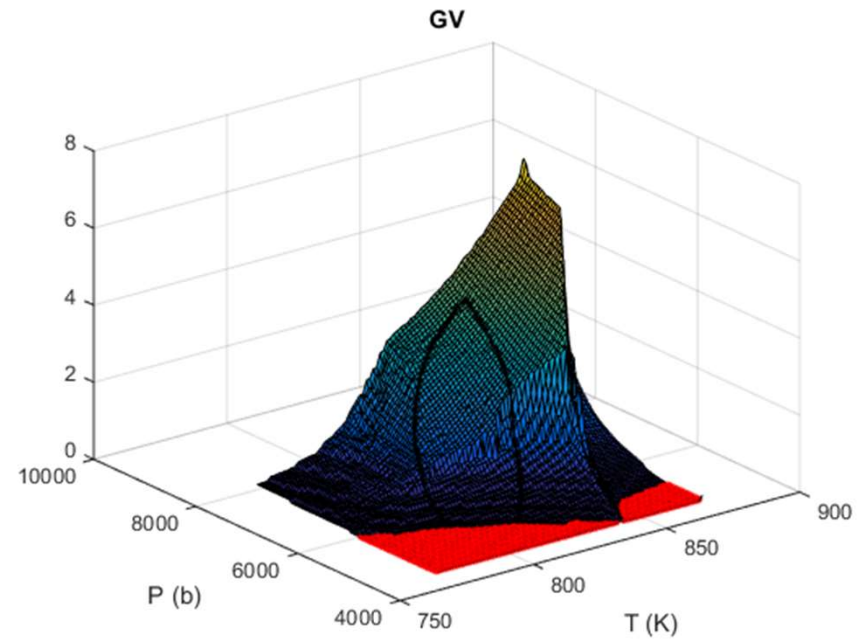
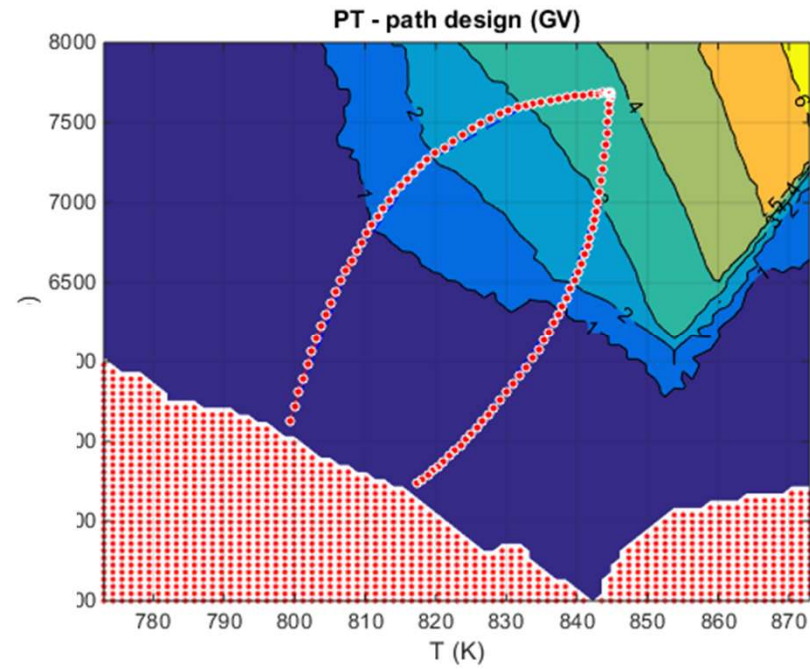
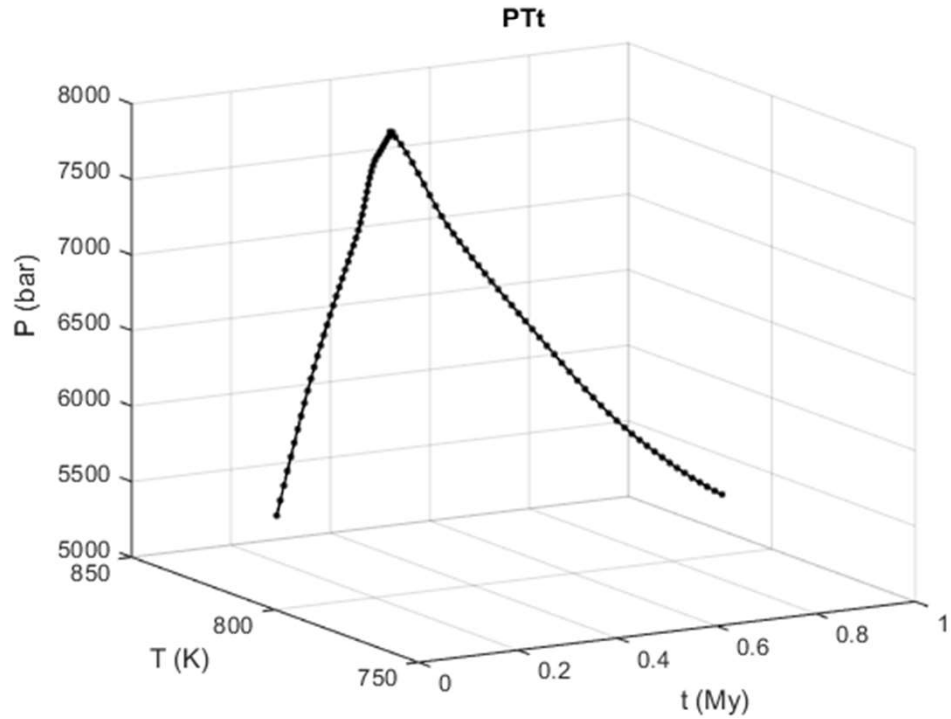
By clicking the **left mouse button** you will select points on the PT grid and by clicking **the right button** you will end the PT path (Fig. a). The program will automatically connect the selected points and draw the PT path (Fig. b).



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

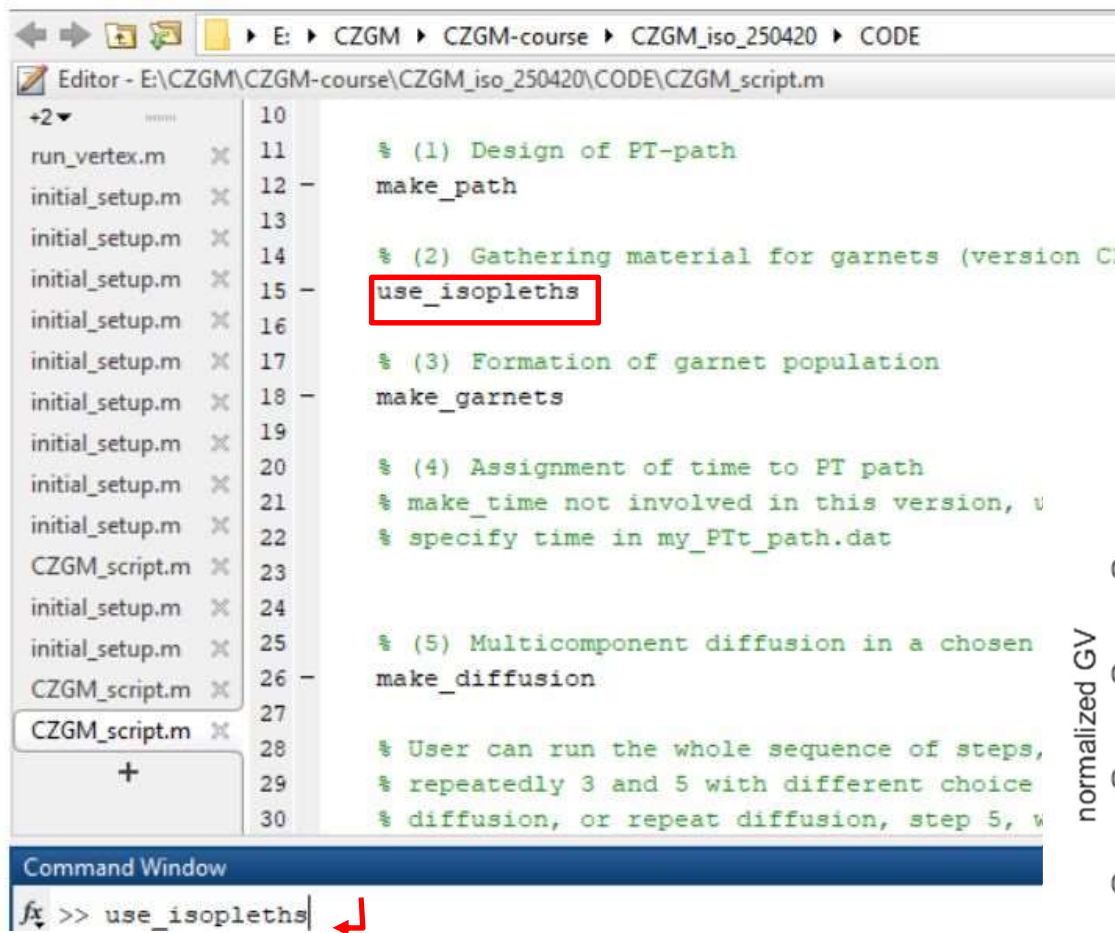


Additional illustrating figures about the PT-t and PT-GV offered by the program:



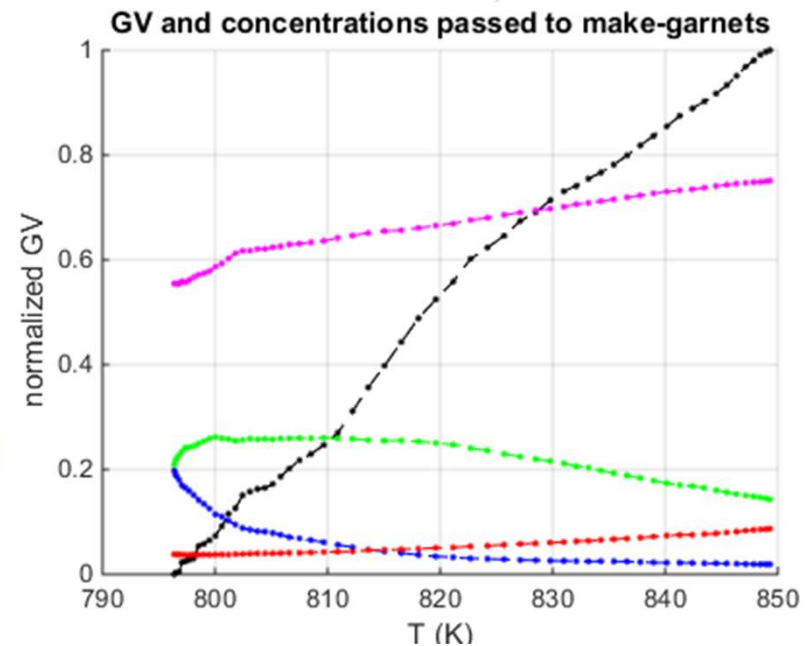
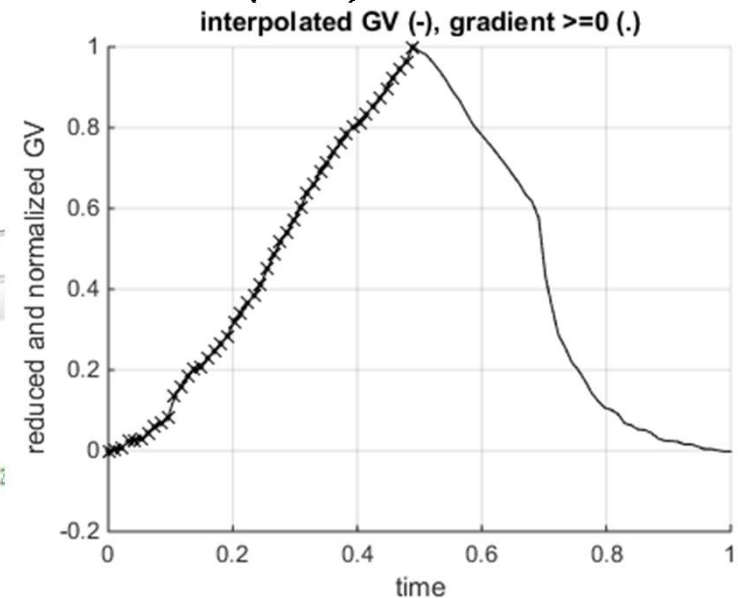
Step 2: use_isopleths

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



```
10
11 % (1) Design of PT-path
12 make_path
13
14 % (2) Gathering material for garnets (version C
15 use_isopleths
16
17 % (3) Formation of garnet population
18 make_garnets
19
20 % (4) Assignment of time to PT path
21 % make_time not involved in this version, v
22 % specify time in my_PTt_path.dat
23
24
25 % (5) Multicomponent diffusion in a chosen
26 make_diffusion
27
28 % User can run the whole sequence of steps,
29 % repeatedly 3 and 5 with different choice
30 % diffusion, or repeat diffusion, step 5, v
```

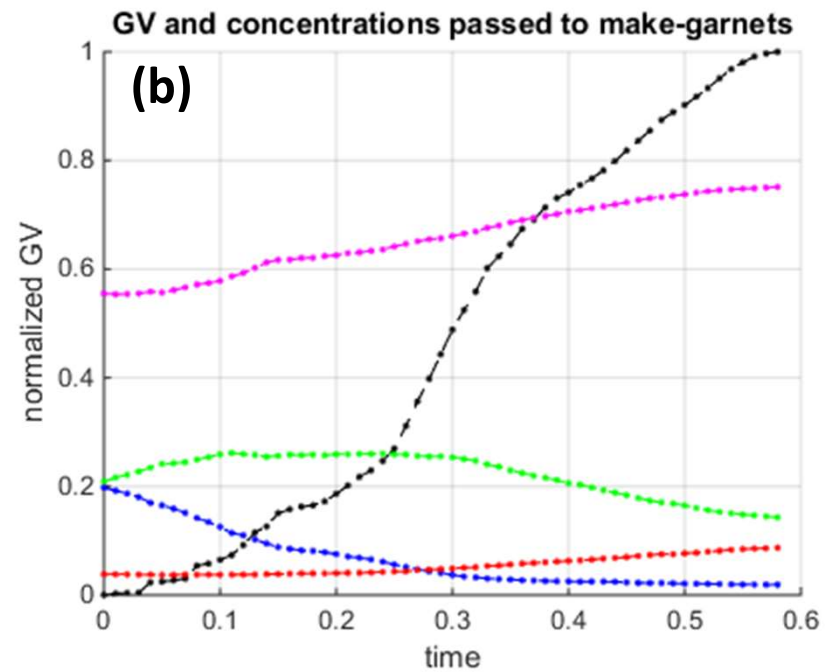
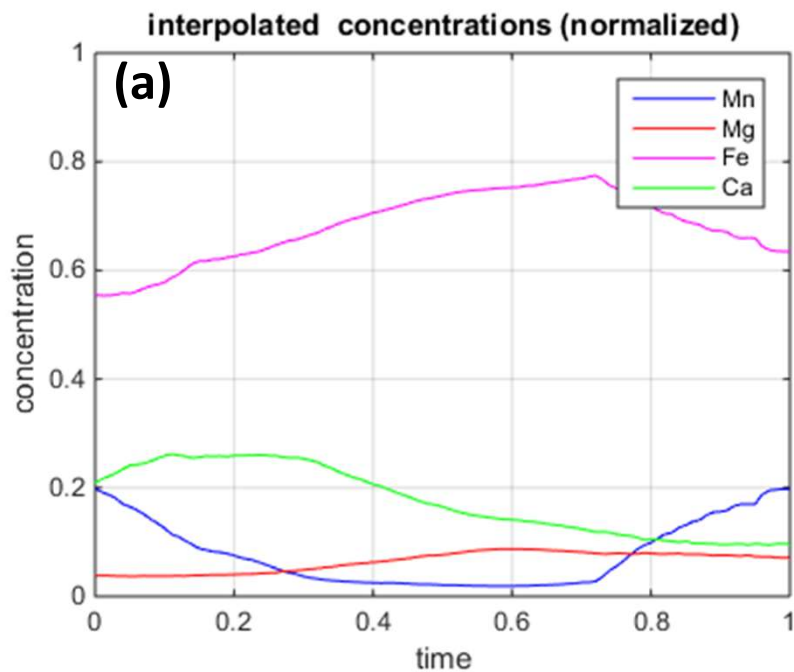
Command Window
fx >> use_isopleths | ↵



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.

```
Editor - E:\CZGM\CZGM-course\CZGM_iso_250420\CODE\CZGM_script
+2
run_vertex.m 10
initial_setup.m 11 % (1) Design of PT-path
initial_setup.m 12 make_path
initial_setup.m 13
initial_setup.m 14 % (2) Gathering material fo
initial_setup.m 15 use_isopleths
initial_setup.m 16
initial_setup.m 17 % (3) Formation of garnet p
initial_setup.m 18 make_garnets
initial_setup.m 19
initial_setup.m 20 % (4) Assignment of time to
initial_setup.m 21 % make_time not involved in
initial_setup.m 22 % specify time in my_PtPa
CZGM_script.m 23
initial_setup.m 24
initial_setup.m 25 % (5) Multicomponent diffus
CZGM_script.m 26 make_diffusion
CZGM_script.m 27
CZGM_script.m 28 % User can run the whole se
CZGM_script.m 29 % repeatedly 3 and 5 with d
CZGM_script.m 30 % diffusion, or repeat diff

Command Window
fx >> make_garnets
```

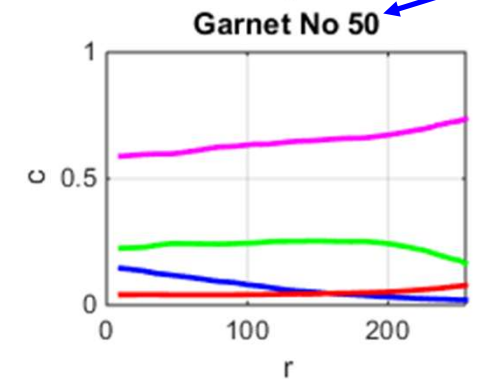
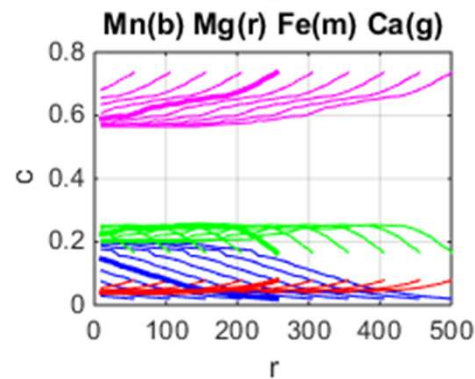
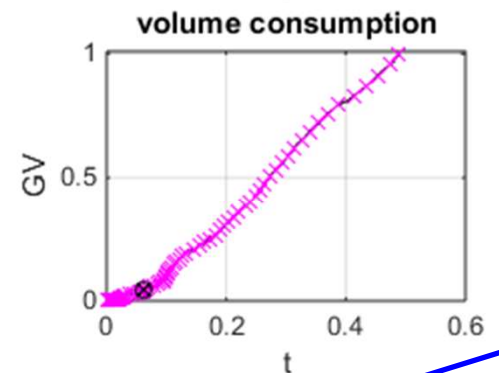
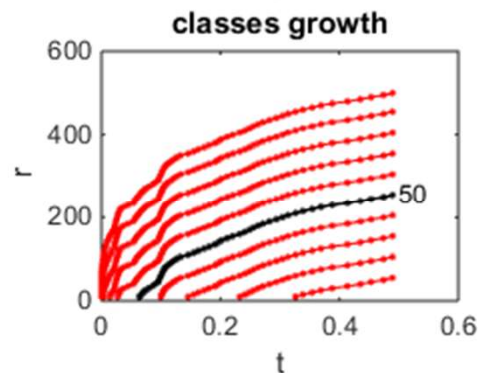
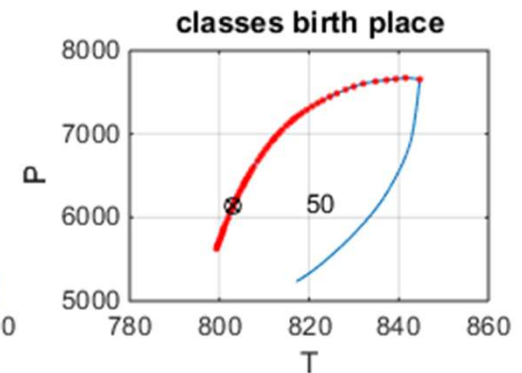
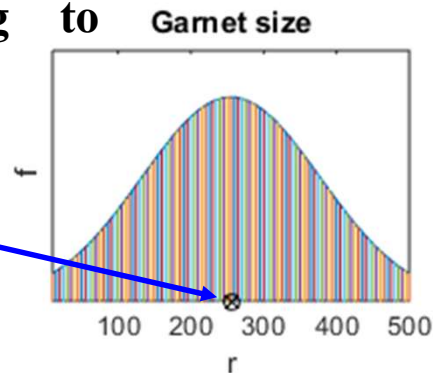
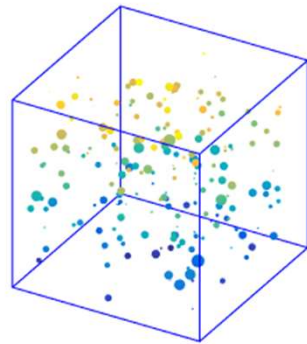


Illustration of initial profile and formation of garnet with time

Garnet size distribution

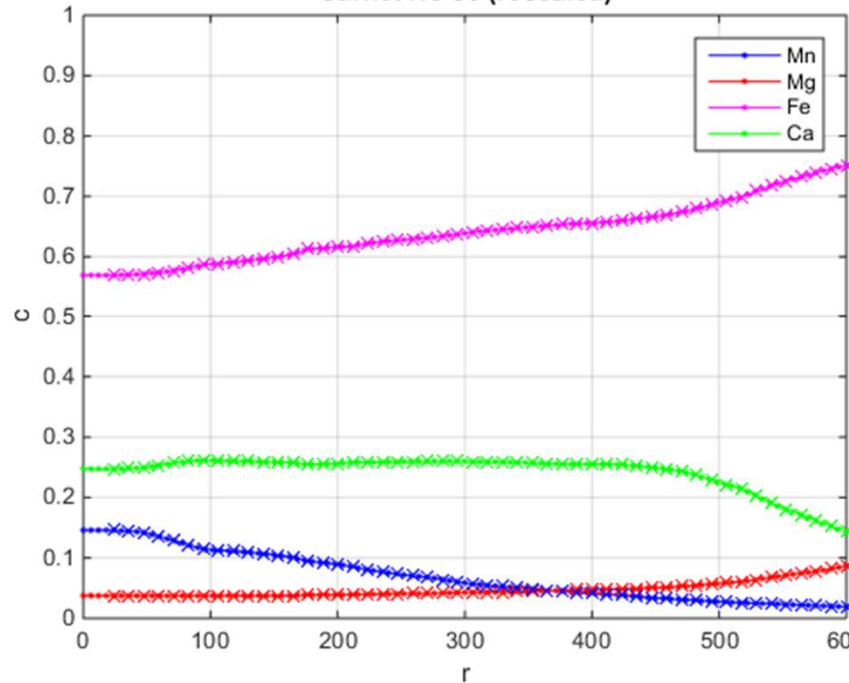


```

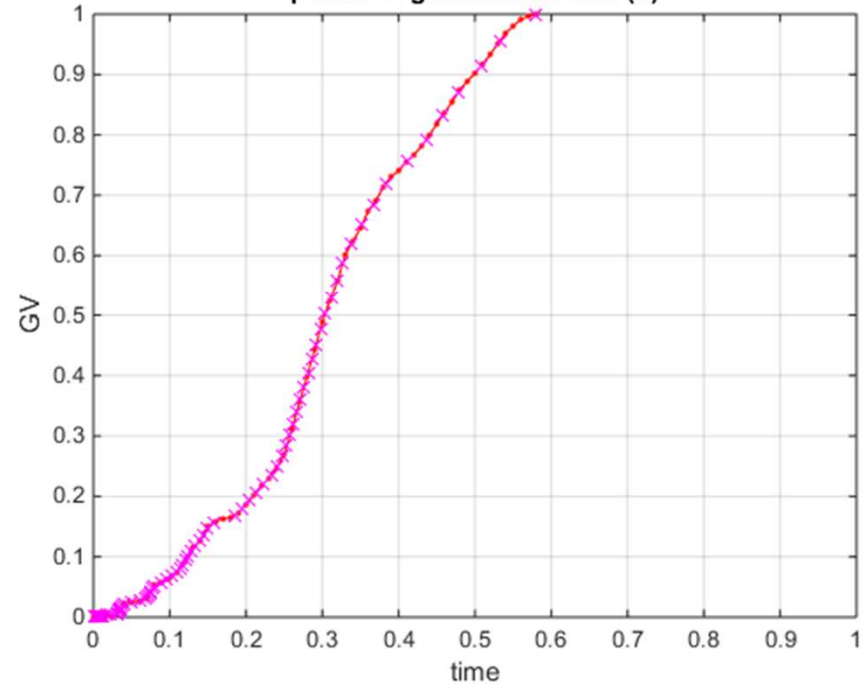
1 % initial_setup
2
3 % Initial setup of parameters and variables for GFDPT
4 % (see CZGM_description for details)
5
6 format compact
7 close all
8 clear all
9 clc
10
11 global data_folder
12
13 global Mn_file Mg_file Fe_file Ca_file GV_file PT_design
14 global min_T max_T min_P max_P
15 global iq_input
16 global n PT
17 global Pi Ti ti % output from make_paths
18 global Mni Mai Fei Cai Gvi % output from make_paths
19
20 global build_file pipe_file
21 global PT_file
22 global ind_Mn ind_Mg ind_Fe ind_Ca
23 global MnG MgG FeG CaG GVG PG TG TG
24 global Mnbn Mgbn Febn Cabn tbu
    
```

Command Window
 New to MATLAB
 >> make_garnet

Garnet No 50 (rescaled)

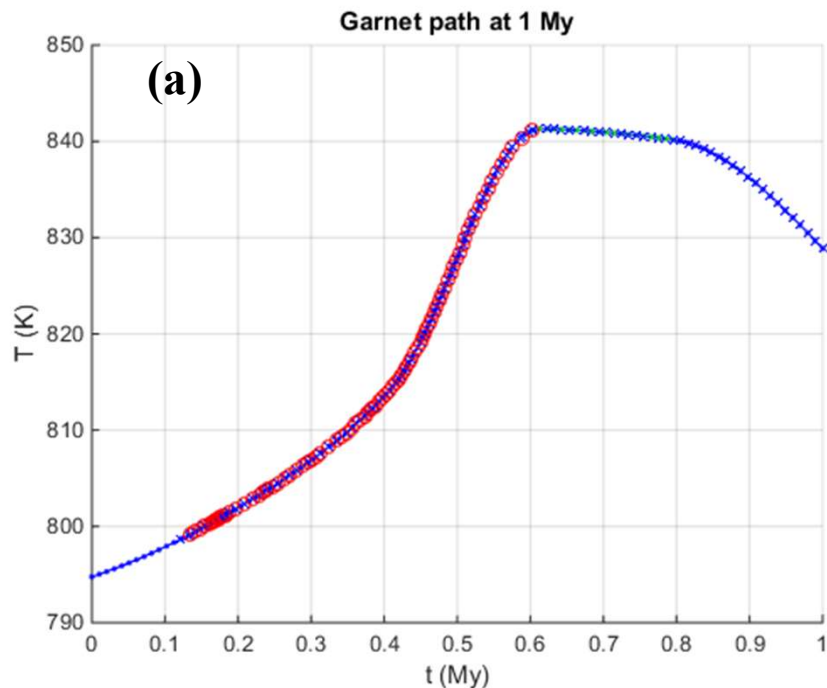


points of garnet formation (x)

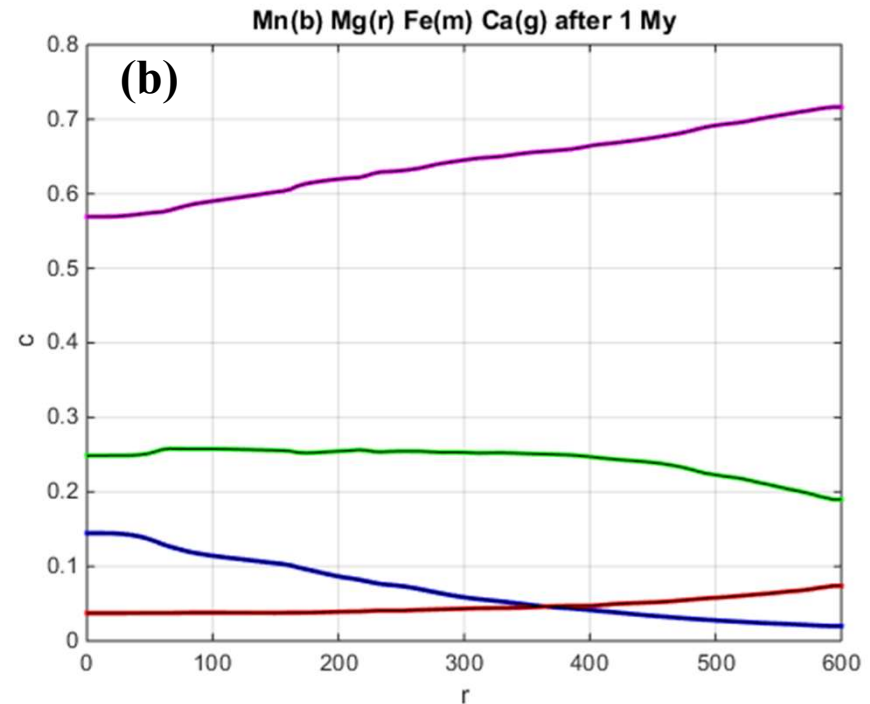
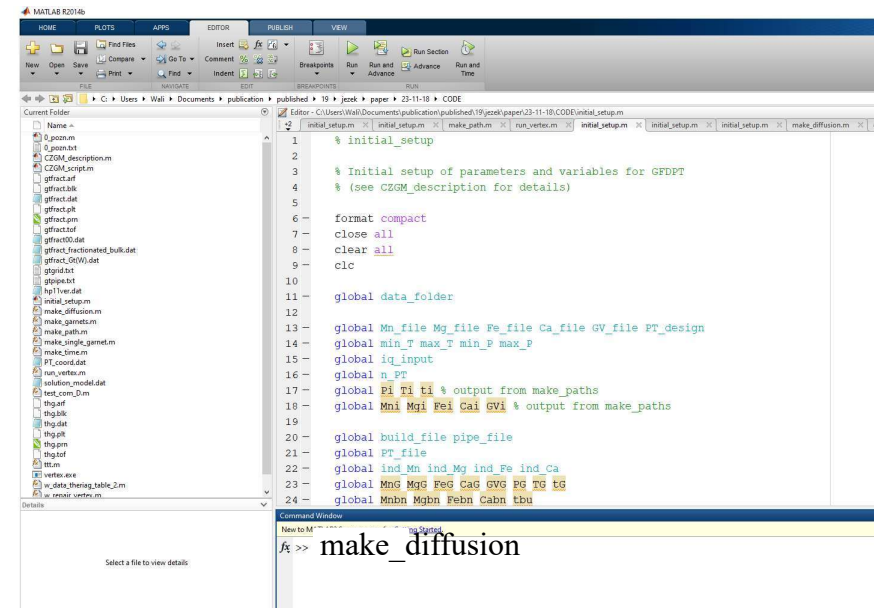


Step 4: make_diffusion

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

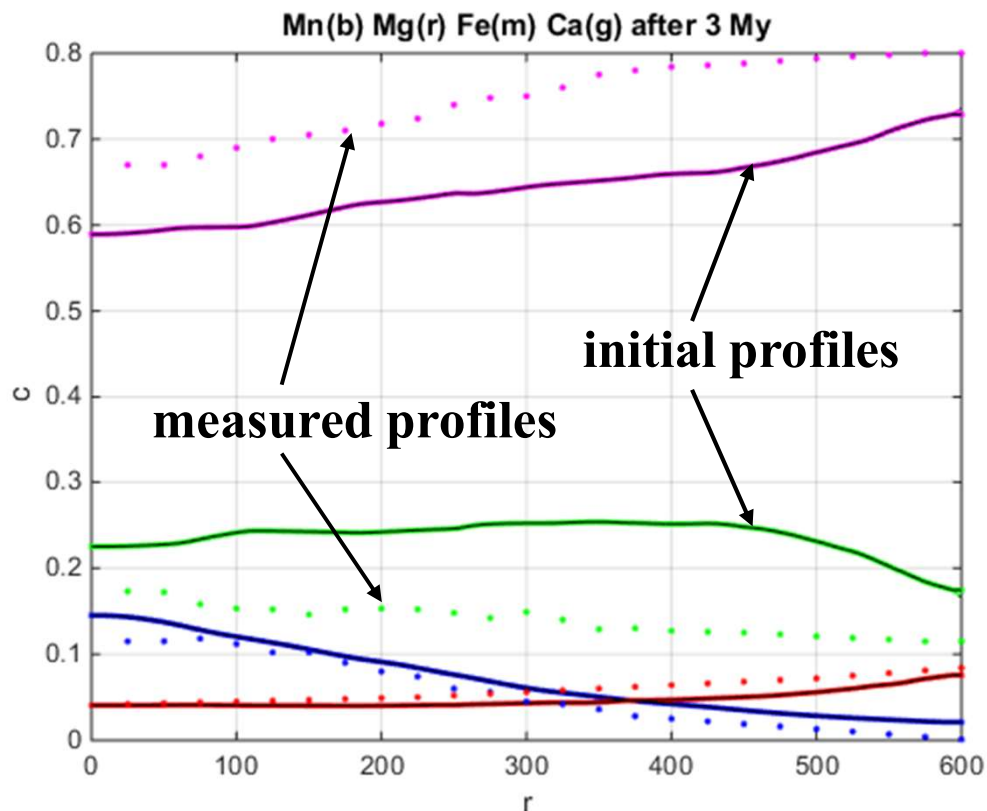
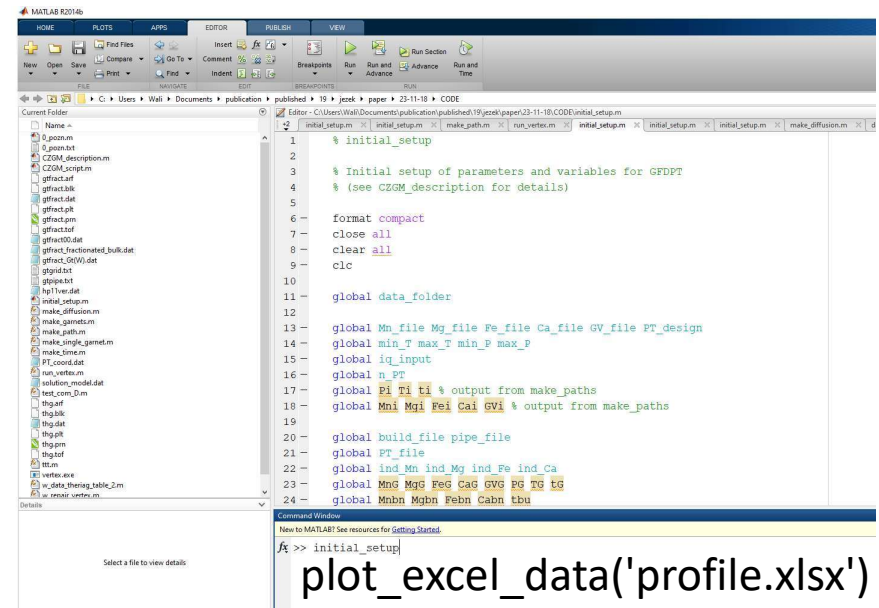


Diffusion of garnet no 50 after 1 Ma



Post-processing: Plotting of measured profiles

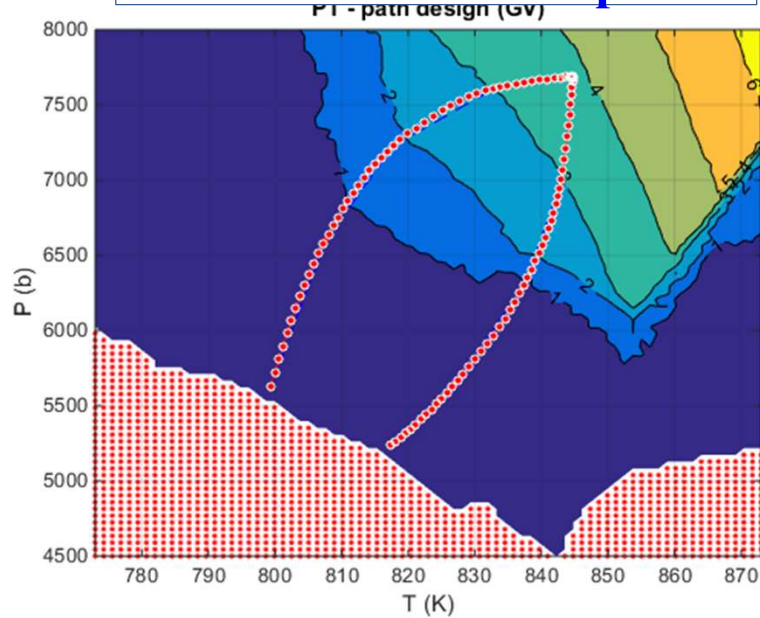
To compare the calculated profiles with that measured, call data from the measured profile in Excel:
`plot_excel_data('profile.xlsx')`



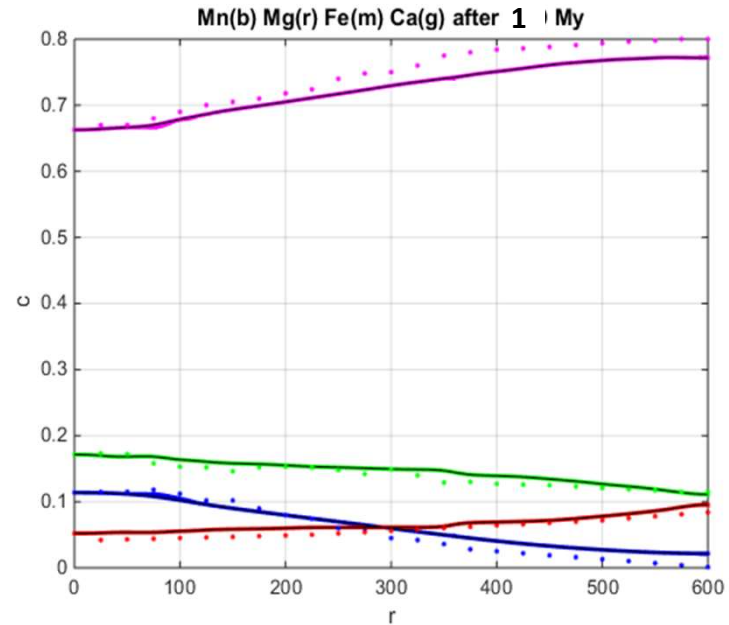
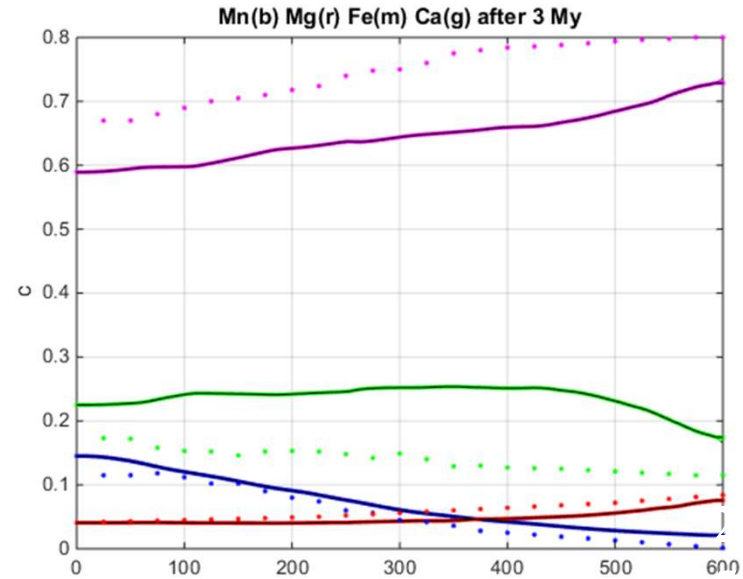
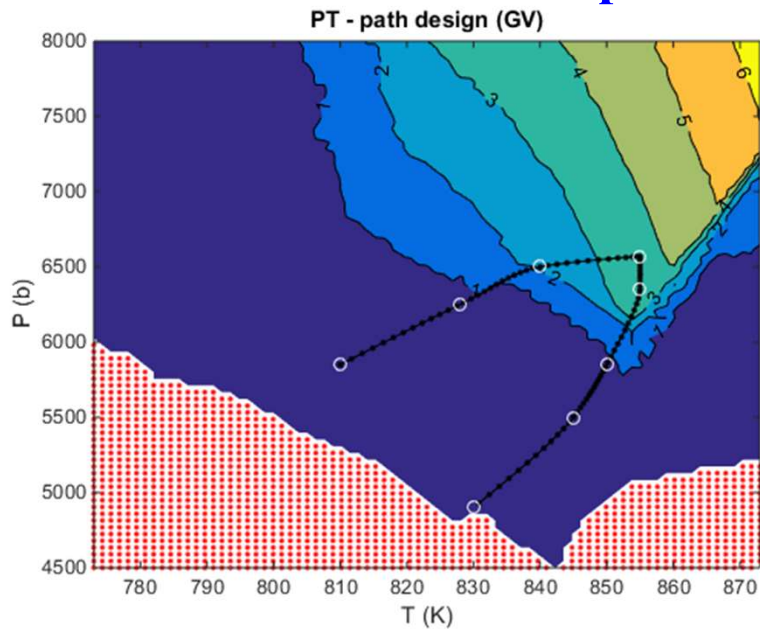
If the modelling was successful, the final (after diffusion) profiles should be close to the measured profiles (dashed lines). As there was no diffusion in the treated garnet, this means the PT path was not correctly selected. We will **continue to try changing the PT path and possibly select another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

Examples from two ad hoc selected and corrected PT paths

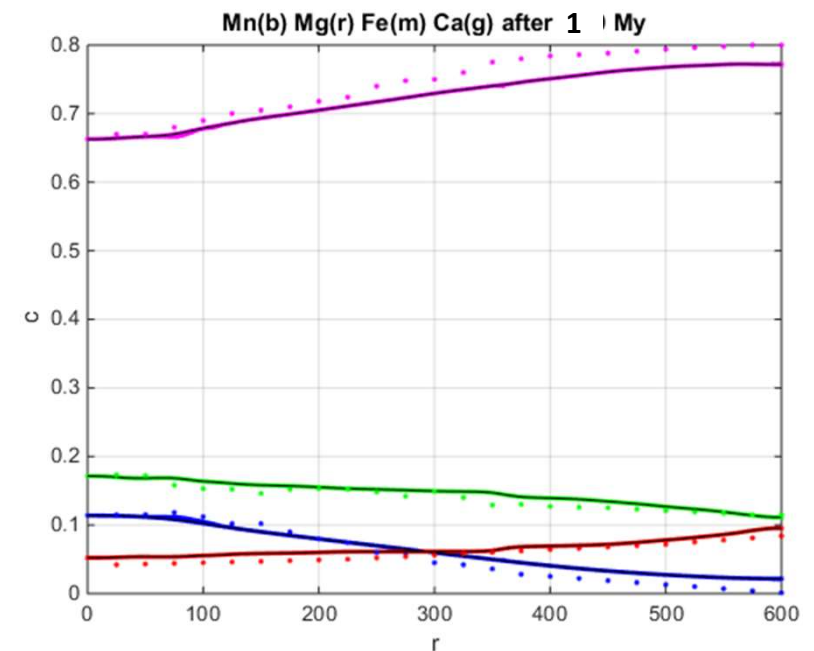
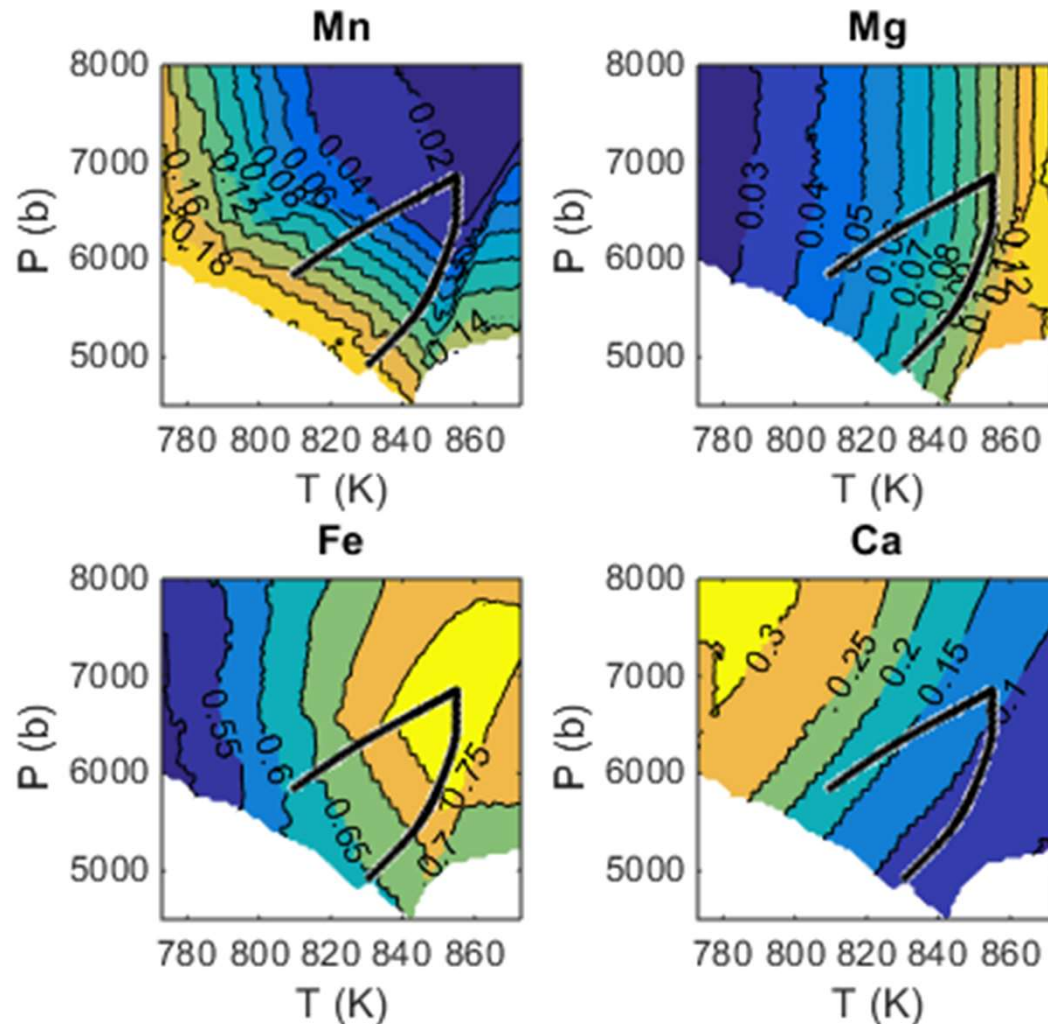
Ad hoc selected PT path



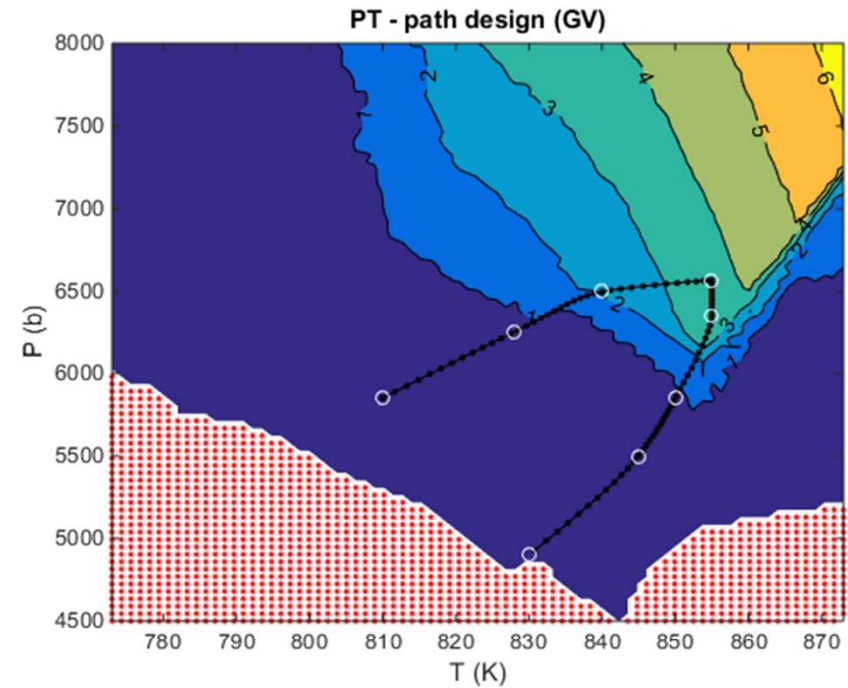
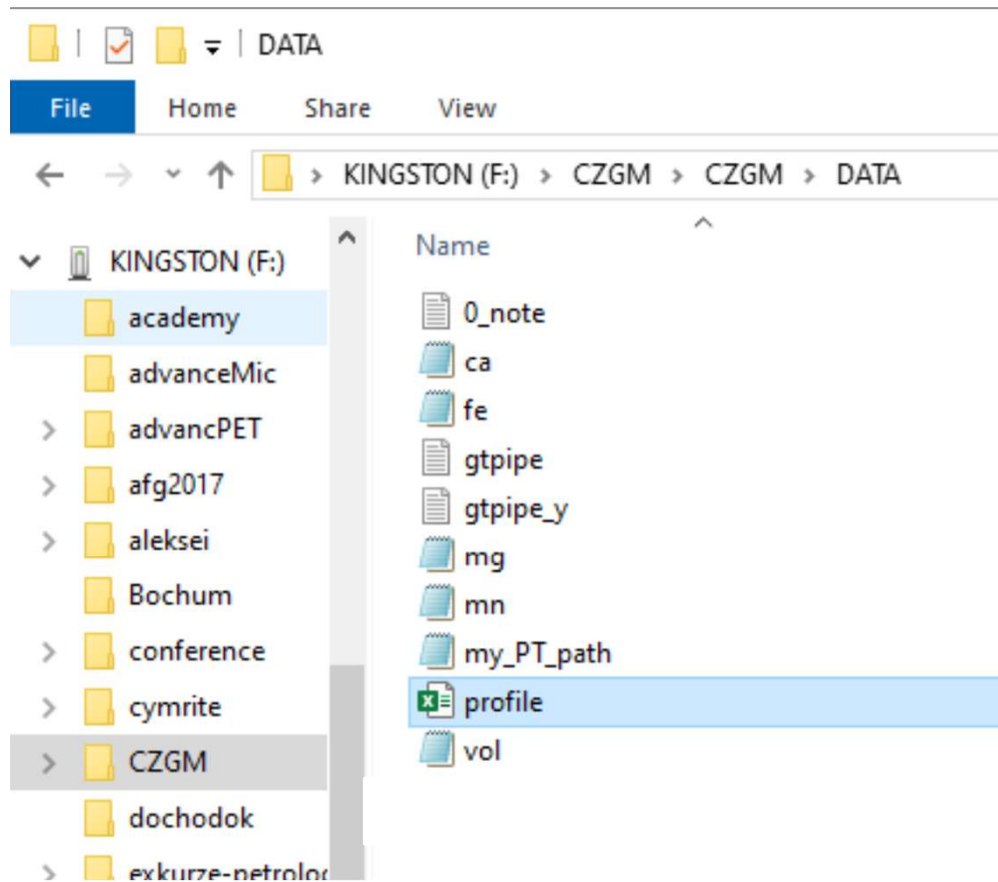
The corrected PT path



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.

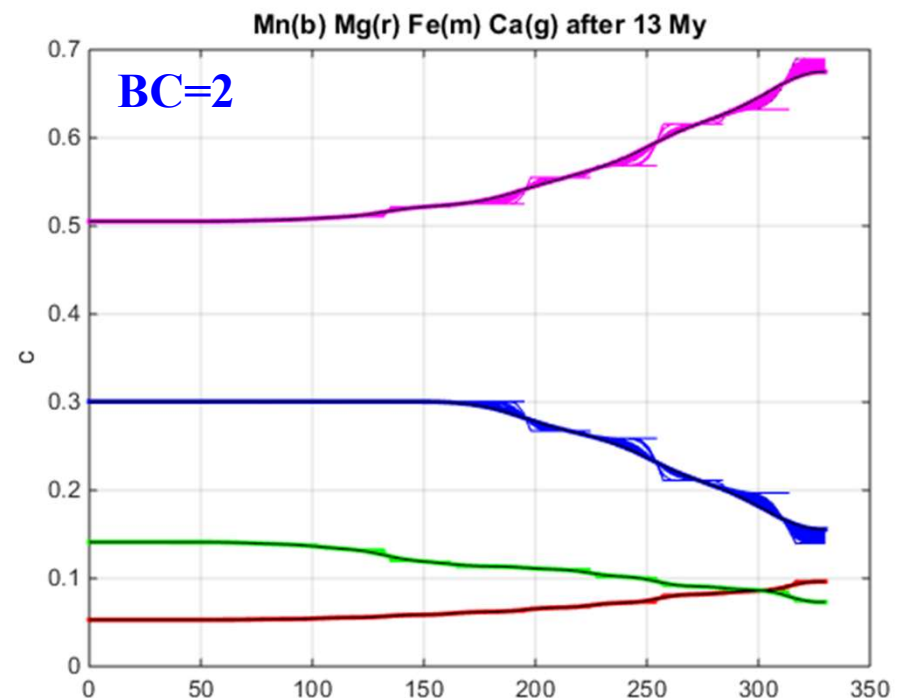
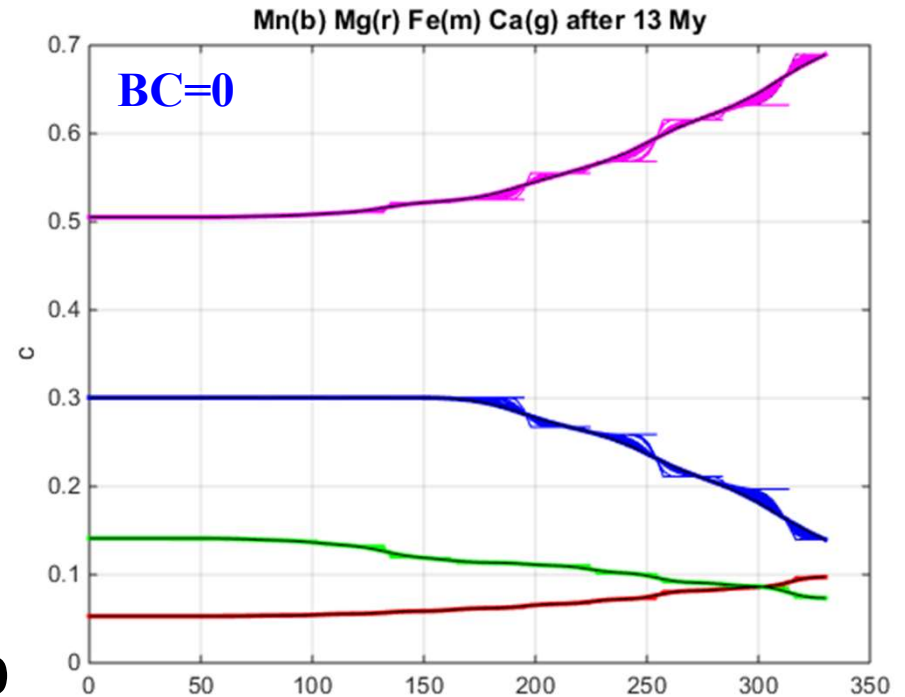
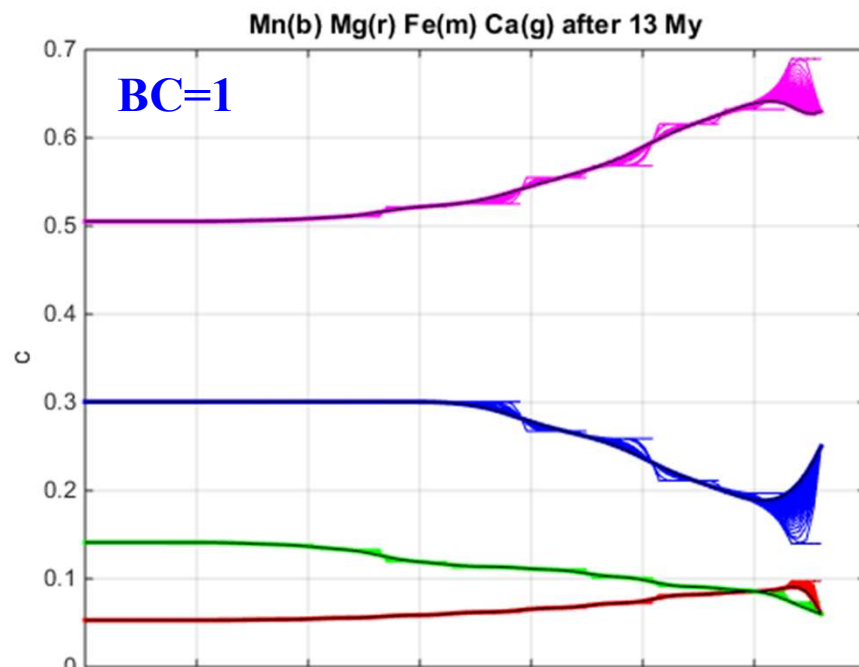
Examples of boundary conditions for the remaining part of the PT-path:

BC=0: fixed boundary concentrations on the garnet rim

BC=1: concentrations defined by user

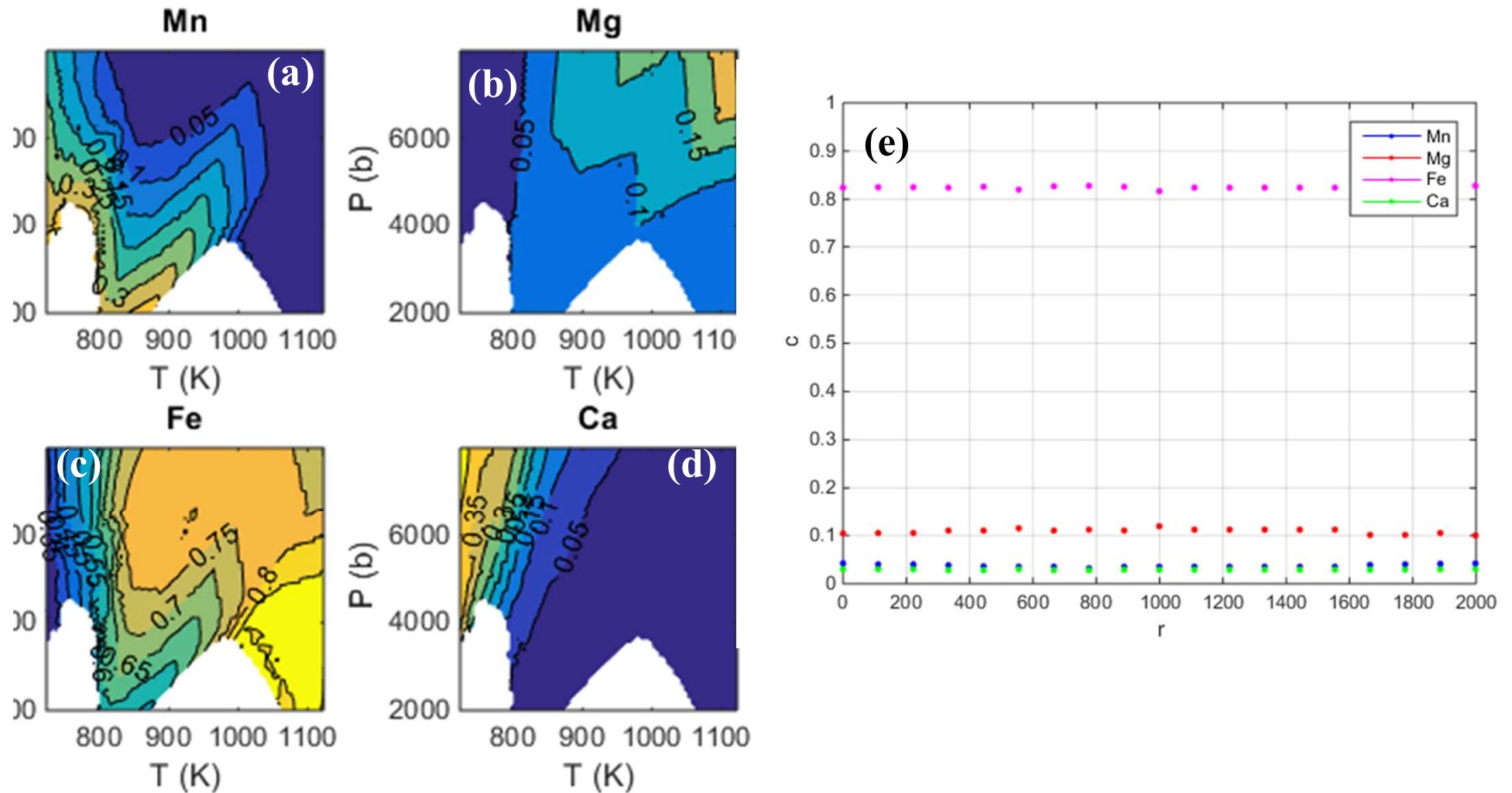
BC=2: closed system (zero gradient)

BC=3: Fe, Mg and Ca interpolated from the PT-grids (isopleths) while Mn=0

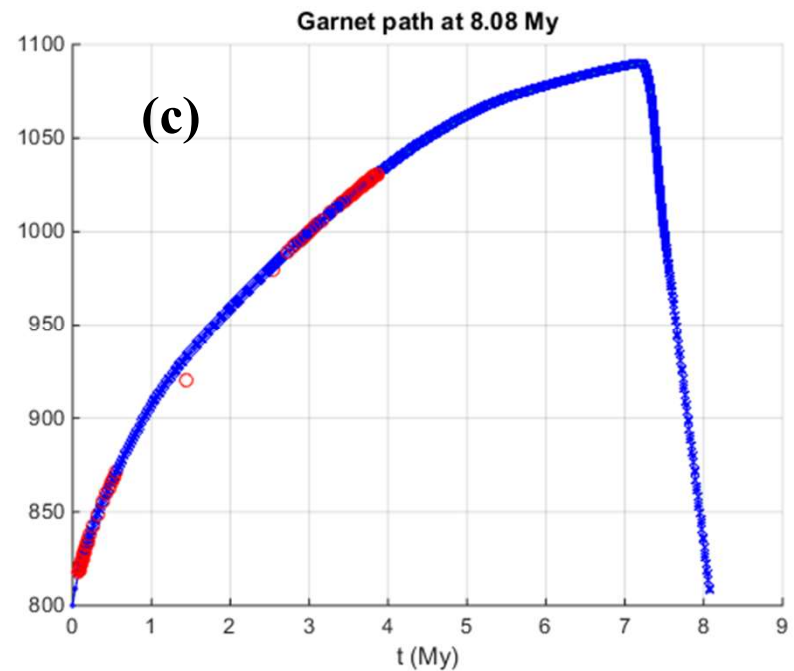
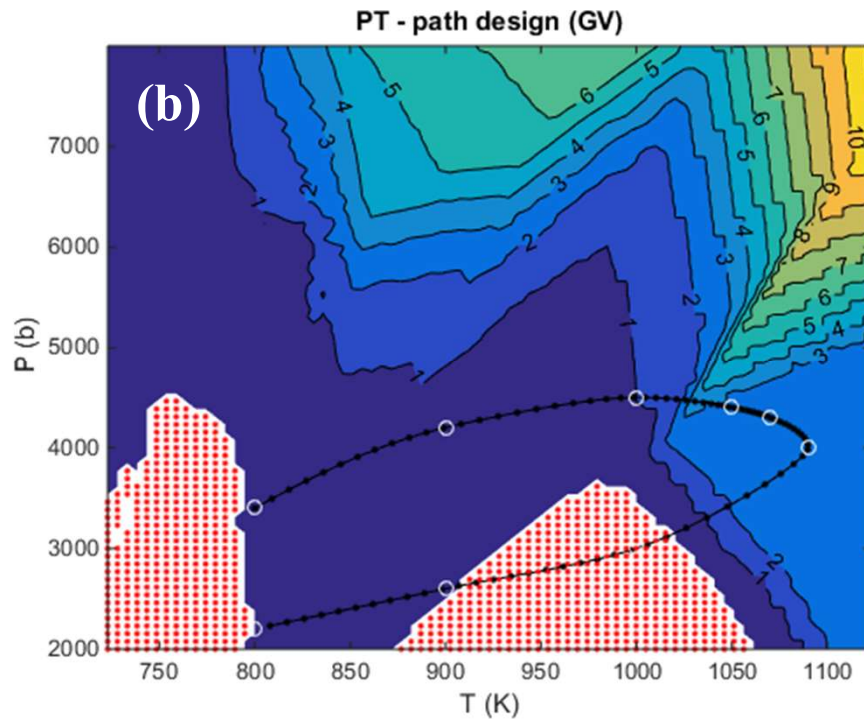
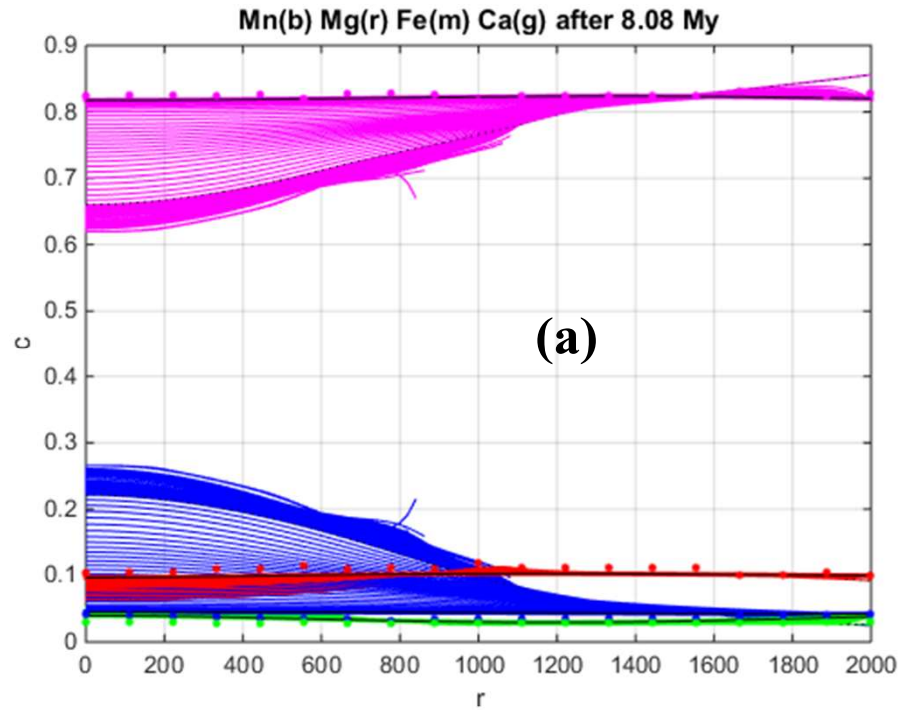


Example of almost homogenized garnet from high-grade terrane

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

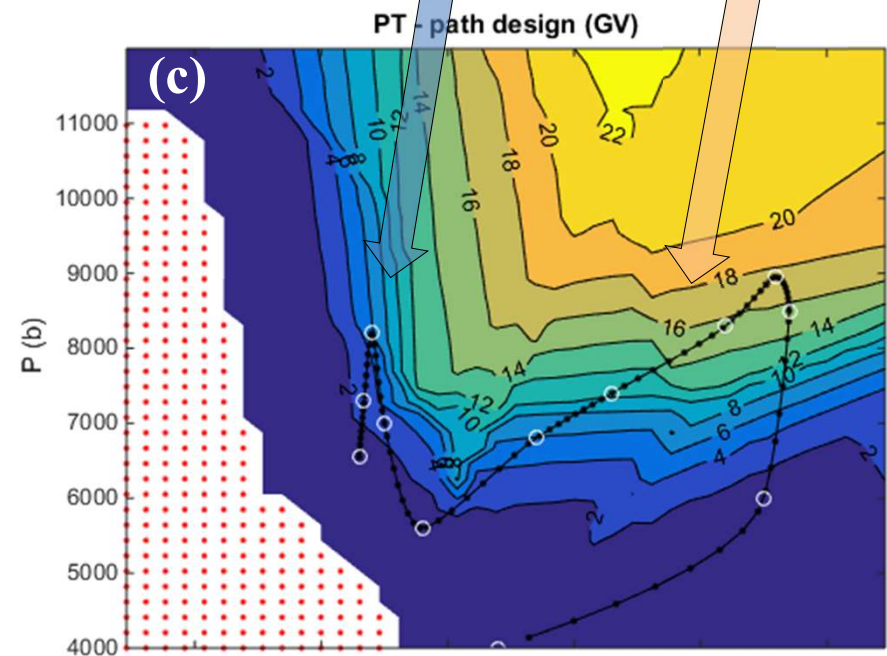
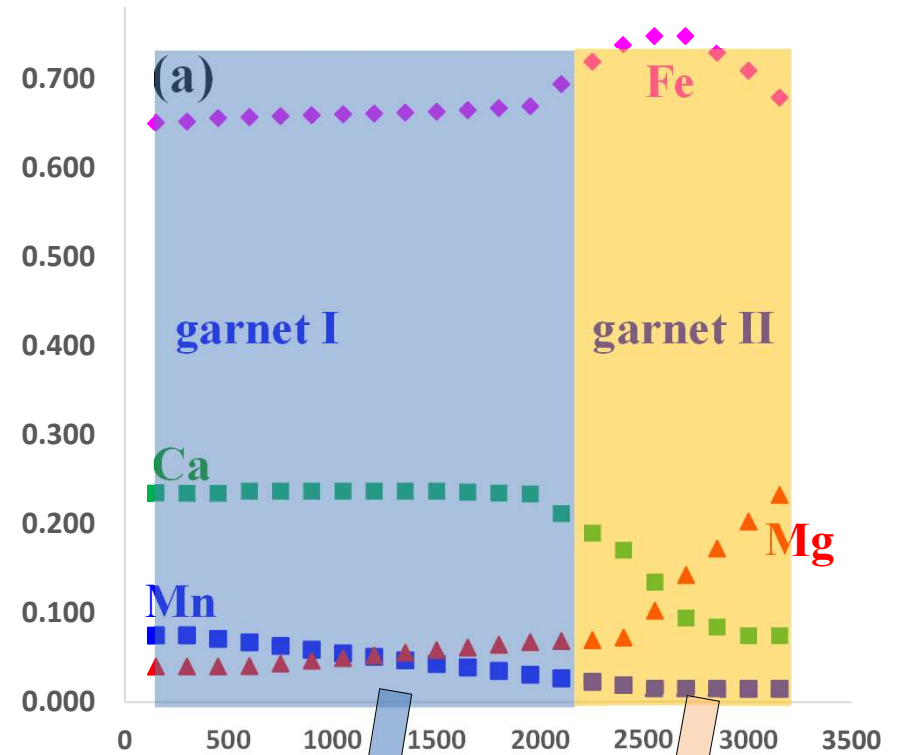
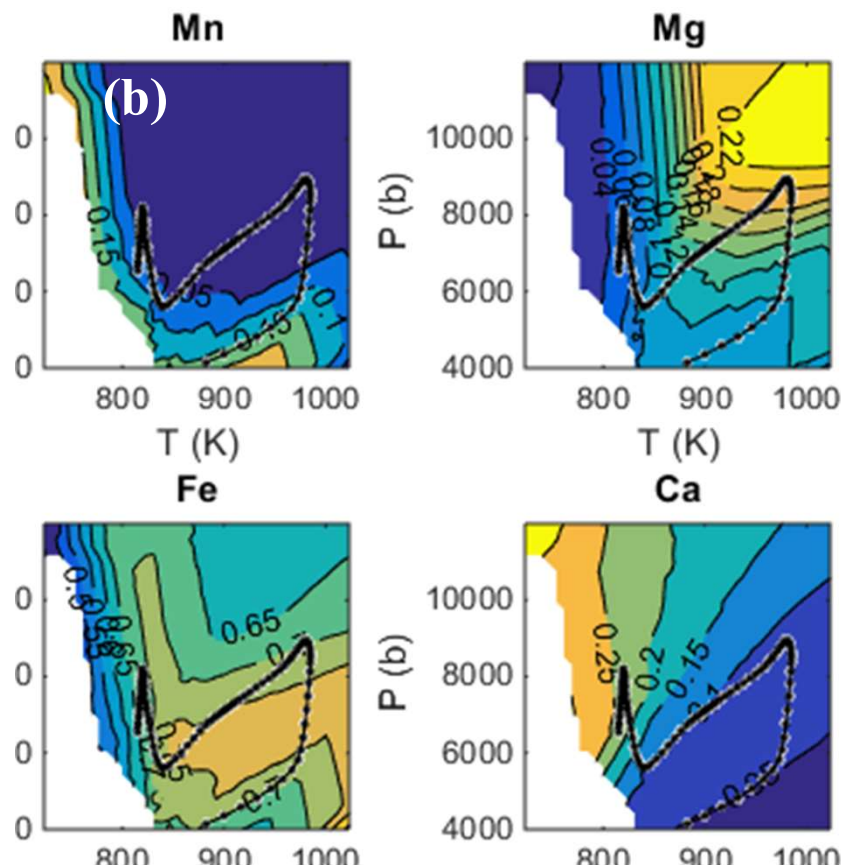


The best fits between measured (dotted) and simulated (lines) profiles (a), obtained for the PT path (b) and time duration (c)



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

