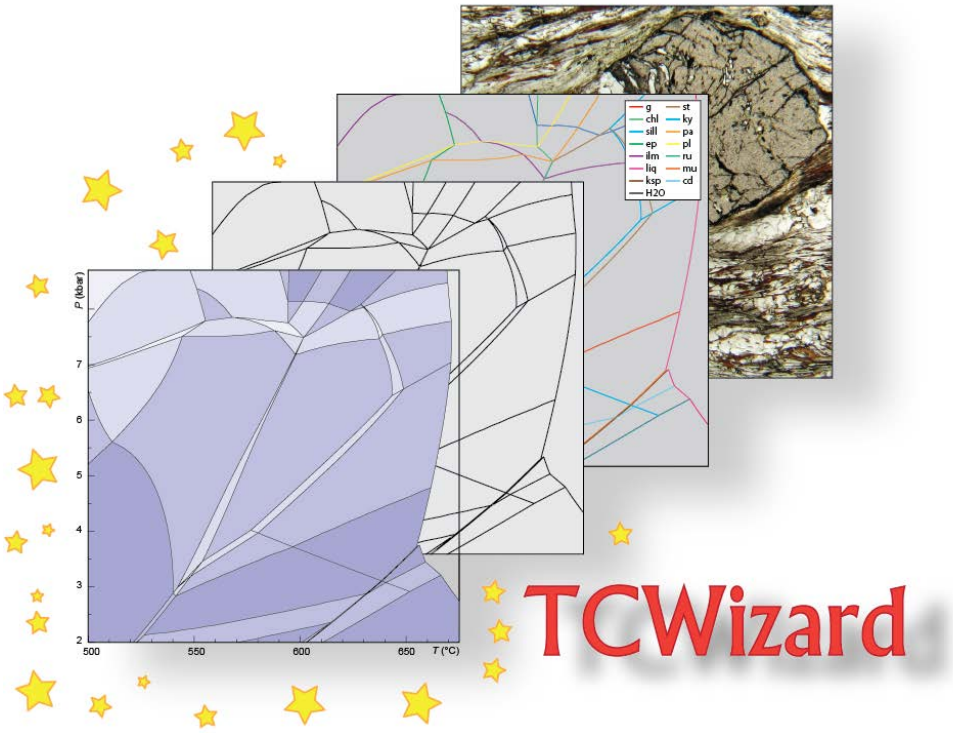
TCWizard Matlab® package

Help File

26/04/2013



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INTRODUCTION

Pseudosections are diagrams representing the stability field of mineral assemblages for a given whole-rock composition, and usually with respect to pressure and temperature. Such P-T pseudosections give valuable information on the stability field of given phases, their modal abundance, or their composition. The P-T pseudosections can be calculated using various programs, among which there is the Thermocalc program (Powell *et al.*, 1998).

TCWizard is a free Matlab® package that provides a graphical interface for the calculation of P-T pseudosections and the handling of data obtained using the Thermocalc program. The main features of TCWizard package involve:

- Quick calculation of single modal or compositional isopleths
- Quick data storage (without interaction with the Thermocalc result text files)
- Simple data management (deleting lines and points, defining begin/end points for lines)
- Display of calculated P-T data
- Interaction with calculated data
- Basic detection of modal or compositional isopleth location
- Calculation of several modal or compositional isopleths at one time
- Automatic definition of begin/end points for lines
- Calculation using Gibbs energy minimization
- Possibility to change starting guess for calculation
- Creation of an output file formatted for drawpd program

TCWizard package can be downloaded from the following webpage:
http://eost.unistra.fr/recherche/ipgs/dylbas/dylbas-perso/benoit-petri/software1/

For reporting troubleshooting or for questions, do not hesitate to contact us:
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1. GETTING STARTED

1.1. TCWizard package

Visit the TCWizard webpage (http://eost.unistra.fr/recherche/ipgs/dylbas/dylbas-perso/benoit-petri/software1/) to download the whole package. The TCWizard package contains:

- **TCWizard** folder with Matlab® files and icons used for the interface
- **tc-example** folder for tutorial
- TCWizard **Help file**

You can extract and save the TCWizard package **anywhere** on your computer or external hard drive. Note that it does not have to be in the same folder as the Thermocalc project.

To **launch** TCWizard:

- Start Matlab® program.
- Set the Current Directory to the path of the **TCWizard folder.**
  - In the Command Window, type **wizz** and press **Enter**.

OR - Open the **wizz.m** file in the Matlab® Editor and press **F5**.

1.2. Preparing Thermocalc files

! IT IS VERY IMPORTANT TO PROPERLY SET UP THE THERMOCALC FILES !

In order to use the TCWizard package, a folder containing Thermocalc files for classical calculations is required. The folder has to contain:

- Thermocalc run file	tc333.exe
- Thermodynamic dataset	tc-ds55.txt
- Project file	tc-example.txt
- a-x model file	tc-MnNCKFMASHTOp&.txt
- Thermocalc preferences	tc-prefs.txt

Preparing the preference file

In the **tc-prefs** file, make sure that:

- the name of the project is correctly specified	scriptfile *example*
- the name of the thermodynamic dataset is correctly specified	dataset *55*
- the calculation mode is set to 1	calcmode *1*

Preparing the project file

The example below shows a Thermocalc project file prepared for the use of TCWizard.

Scripts in red are mandatory.

Scripts in blue are optional.

---

axfile *(ex: MnNCKFMASHTOp&)* — **a-x file used for calculations**

```
infolevel 1
```

ignore *(ex: ged opx)* — **List of phases ignored for calculation, optional**

printxyz yes — **| Scripts to print**
printguessform yes — **| mineral compositions**
printbulkinfo yes — **| in the tc-log file (yes)**

setexcess *(ex: q mu)* — **List of excess phases, optional**

calctatp ask — **Ask if calculate P at T or T and P (ask)**

setdefTwindow yes 400 800 — **Default T range (yes Tmin Tmax)**
setdefPwindow yes 1 10 — **Default P range (yes Pmin Pmax)**

```
project no

seta no
```

setiso yes — **Compositional isopleth calculation (yes)**

pseudosection yes

```
% ------------------------------------------------------------------------
% EXAMPLE COMPOSITION
%            SiO2   Al2O3  CaO   MgO   FeO   K2O   Na2O   TiO2   MnO   O
setbulk yes  70.89  10.81  0.74  3.35  5.12  2.53  1.05   0.68   0.07  0.03
% ------------------------------------------------------------------------
```

setmodeiso yes — **Modal isopleth calculation (yes)**
zeromodeiso no — **Zero-mode calculation (no)**

dogmin no — **Do Gibbs energy minimization (no)**

drawpd yes — **Write calculation results in tc-*example*-dr (yes)**

```
*
```

Structure of the project file

For more information on the different scripts, please visit

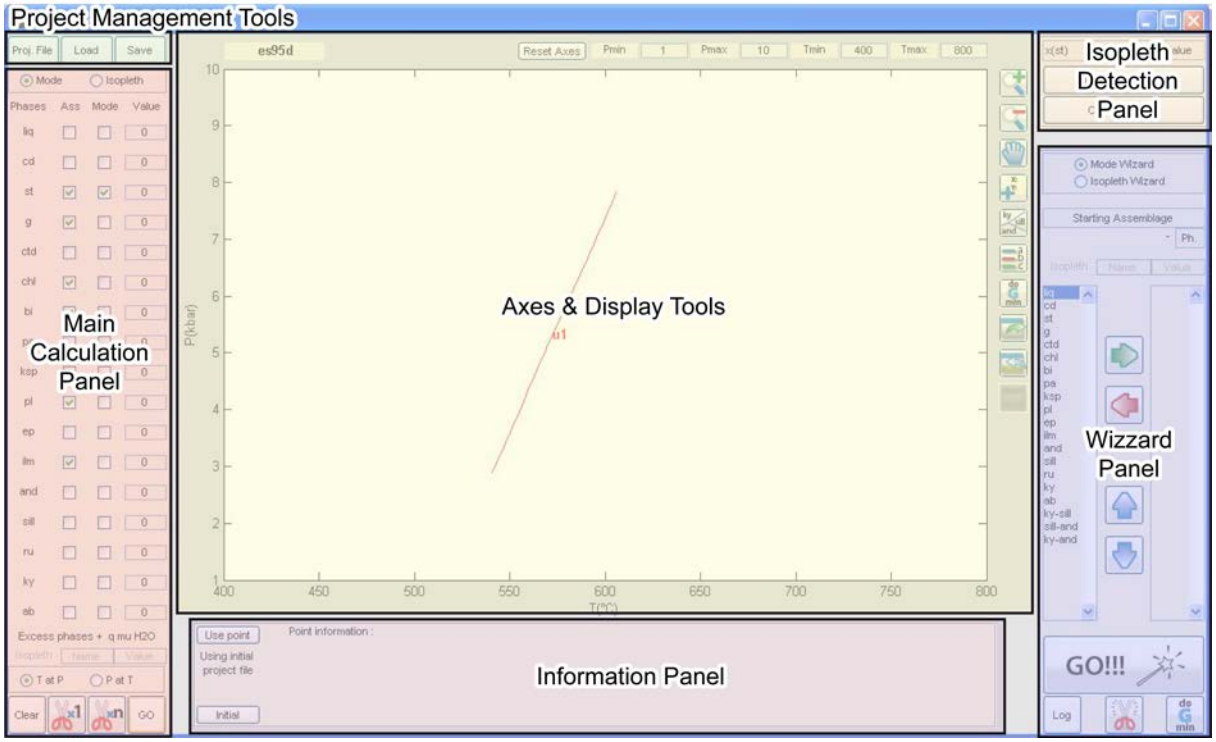
http://www.metamorph.geo.uni-mainz.de/thermocalc/documentation/scripts/index.html

2. TCWIZARD INTERFACE

2.1. Overview

The TCWizard interface is composed of several panels.

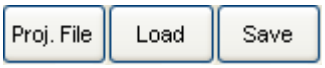
- Project Management Tools
- Main Calculation Panel
- Axes & Display Tools
- Information Panel
- Isopleth Detection Panel
- Wizard Panel

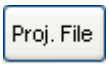


TCWizard interface

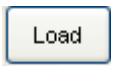
2.2. Project Management Tools

The Project Management Tools are used to select a project file that will be used by Thermocalc, and to Load/Save calculated data.

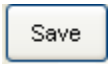




• **Proj. File** Display a dialog box to select the project file (tc-*projectname*.txt)



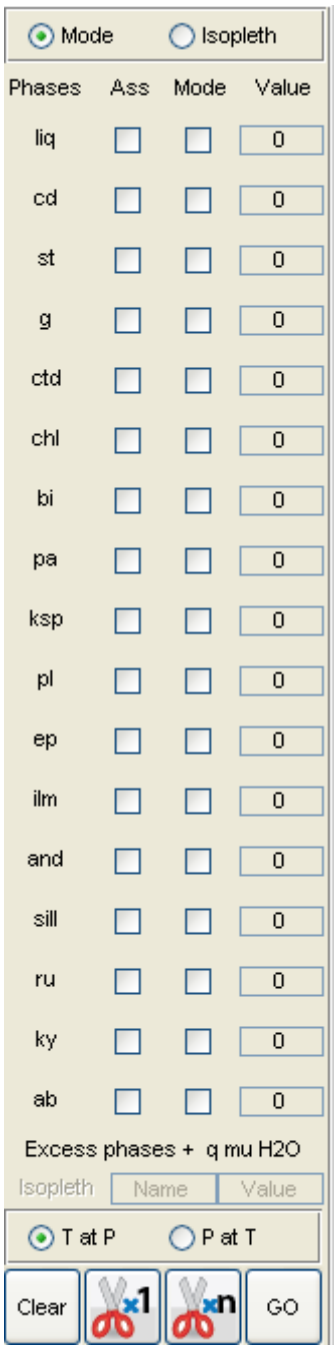
• **Load** Display a dialog box to load existing results stored in a Matlab data file (.mat)



• **Save** Display a dialog box to save calculation results into a user's selected Matlab data file (.mat)

2.3. Main Calculation Panel

The Main Calculation Panel comprises an initial choice for the calculation of **Modal isopleths (Mode)** or **Compositional isopleths (Isopleth)**.



Upon choice of a project file, the Panel displays:

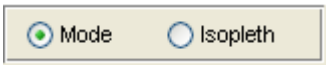
- the **list of phases** available for calculation (without excess and ignored phases),
- checkboxes to choose the **assemblage**,
- checkboxes to choose the **phase(s)** for which the **modal isopleth** will be calculated,
- edit text boxes to type the calculated **mode value(s)**,
- the list of **excess phases**.

If compositional isopleths are calculated, the **isopleth name** and **value** are required in two edit text boxes.

There is also the possibility to calculate **pressure** at given **temperature** intervals or temperature at given pressure intervals (Thermocalc “calculate P at T question”).

The different buttons at the bottom of the Panel allow to:

- **clear** calculated and displayed results,
- **cut lines** according to begin/end points,
- **launch** Thermocalc calculation.



• **Mode/Isopleth** Choose Modal or Compositional isopleth calculation
(default - Modal isopleth calculation)

• **Assemblage** Check box if the corresponding phase is part of the calculated assemblage.
(default - unchecked)

• **Mode** Check box if a modal isopleth for the corresponding phase has to be calculated.
Note: Assemblage has to be checked for that phase.
(default - unchecked)

• **Value** Enter the modal isopleth value that has to be calculated for the corresponding phase.
Note: Mode and Assemblage have to be checked for that phase.
(default - 0)

If compositional isopleth calculation is selected

• **Name** Enter the name of the compositional isopleth that has to be calculated.
(ex: x(st))

• **Value** Enter the value of the compositional isopleth that has to be calculated.
(ex: 0.88)

• **T at P / P at T** Calculate temperature at given pressure intervals or pressure at given temperature intervals.
(default - T at P)

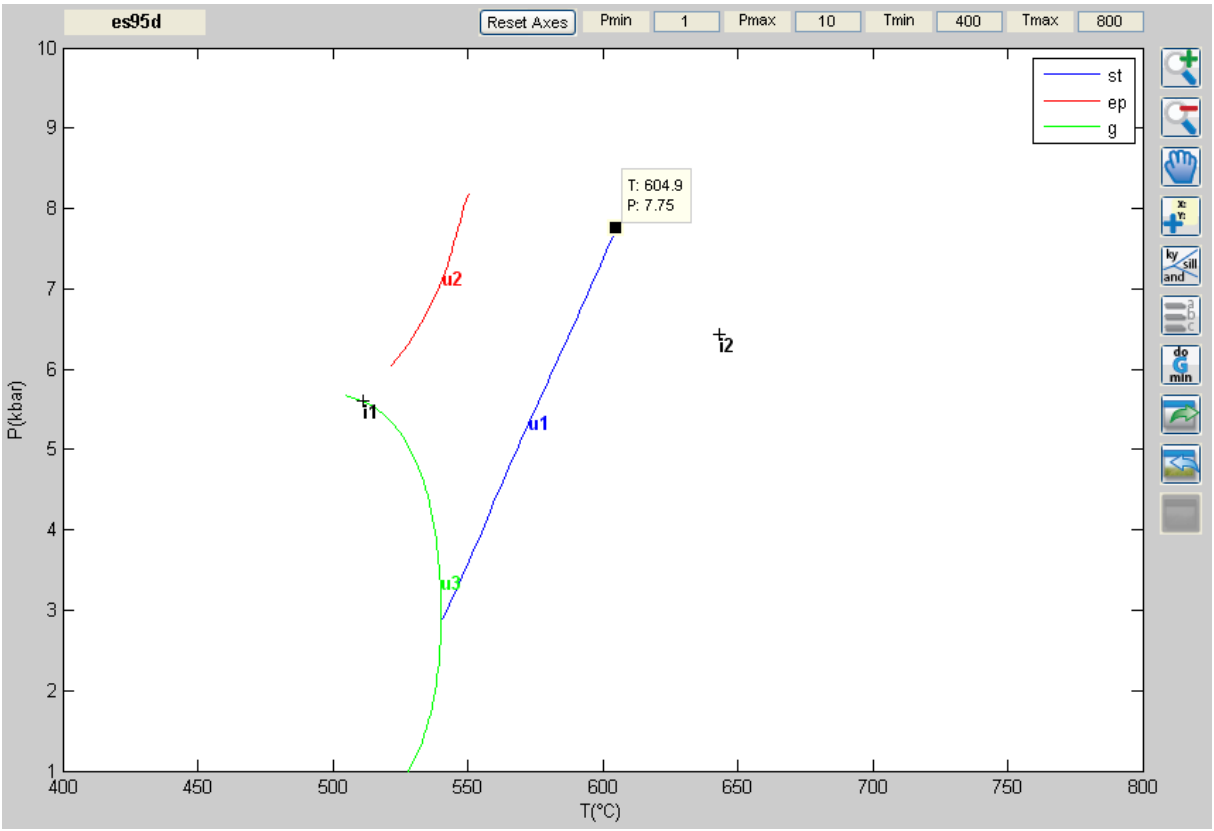
• **Clear** Clear a calculated line or point and delete it from the axes. Display a first menu to clear either a line or a point. Display a second menu to select the line/point to be deleted according to its number. See also 3.5. Clear a line/point.

• **Cut x1** Cut a selected line according to “begin/end” point(s). Display a first menu to select the line to be cut. Display then two successive menus to select the “begin” and “end” points. See also 3.6. Cut a line.

• **Cut xn** Cut lines according to “begin/end” point(s). Same as **Cut x1**, but successively ask for all existing lines that have not been previously cut. See also 3.6. Cut a line.

• **GO** Launch Thermocalc calculation. For lines, an hourglass will replace the “GO” button until the calculation is finished. For points, the calculation is almost immediate.

2.4. Axes & Display Tools

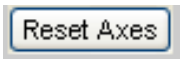


Axes and display tools

The P-T axes are used to display the different results from Thermocalc calculations. It is possible to display: modal isopleths, compositional isopleths, points, compositional isopleth detection, or results of Gibbs energy minimization. In addition, a background image can be displayed. Several display tools are available next to the axes.

• **Project name** Once a project file is chosen, display the name of the current project. It corresponds to the suffix of the project file (tc-*projectname*.txt).

• **P-T range** Edit text boxes to change the P-T range. The new P-T limits are used for calculations and display as long as they are not changed or reset. Note: these P-T limits do not delete the default P-T range specified in the project file.
(default - P-T range specified in the project file by the scripts setdefTwindow yes/setdefPwindow yes)



• **Reset Axes** Reset axes limits to the default P-T range specified in the project file.

• **Zoom In** Zoom in on a selected region of the axes.

• **Zoom Out** Zoom out from a selected region of the axes.

• **Pan** Pan the view of the axes.

• **Data Cursor** Switch on data cursor to get point information (see 2.5. Information Panel).

• **Show/Hide and-ky-sill** Show/hide the Al_2SiO_5 phase diagram. The diagram is added to the displayed data.

• **Show/Hide legend** Show/hide the legend. The legend contains the color coding of the different lines according to the phase out.

• **Show/Hide Dogmin results** Show/hide the results of Gibbs energy minimization. The results are added to the displayed data. See also 3.11. Gibbs energy minimization.

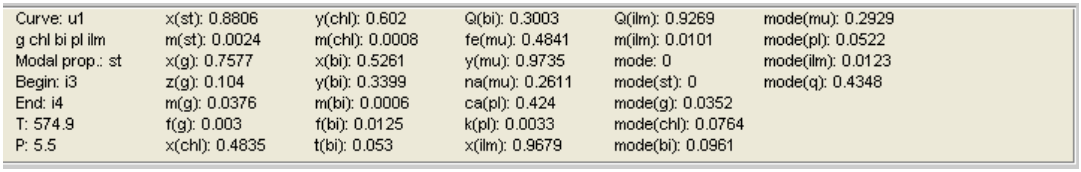
• **Export figure** Export the current axes to a figure file. Available formats are:
color EPS (.epsc), JPEG (.jpg), TIFF (.tif), Adobe Illustrator (.ai).

• **Import background image** Import a background image in the axes. Two successive dialog boxes will ask for the P-T coordinates of the image edges. See also 3.9. Import a background image.

• **Show/Hide background image** Show or hide the background image.

2.5. Information Panel

The information panel allows to visualize the properties of any calculated point. Any selected point can further be used to perform new calculations using its compositional data (see also 3.10. Use new starting guess).



• **Information** Display information about the selected point. Available information:

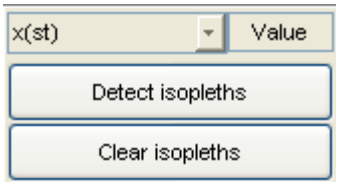
- Object type (Curve/Point)
- Assemblage
- Phase name for modal proportion calculation / Isopleth name
- “Begin” and “End” points (if specified)
- P-T coordinates
- Compositional isopleth data
- Modal isopleth data
- Number of the dogmin data point (if dogmin used)

• **Use point** Use the compositional data of a point selected with the data cursor for calculations. Display in the information panel the coordinates and host line of the selected point. (Warning ! The new ptguess are saved in the original project file).

• **Initial** Use the initial compositional data for calculations. Reset the compositional data of a previously selected point.

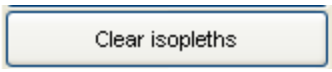
2.6. Isopleth Detection Panel

The Isopleth Detection Panel can be used to spot the approximate location and trend of modal or compositional isopleths between already calculated lines.



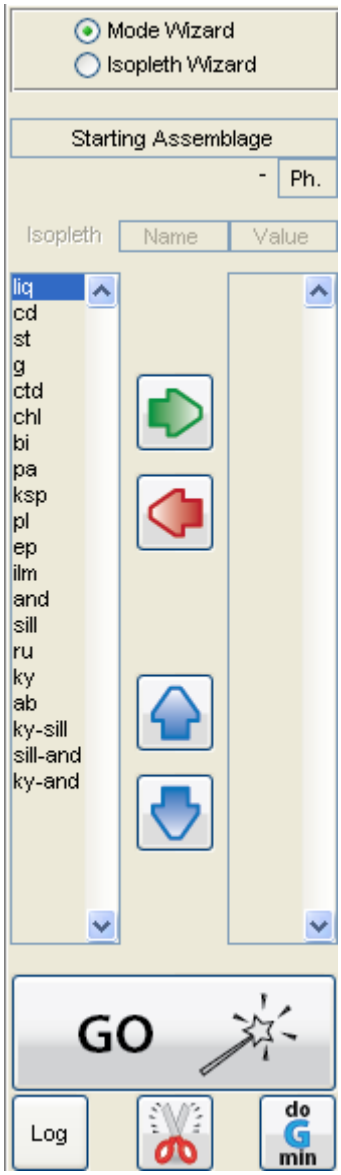
• **Isopleth name/value** Select the name and value of the modal or compositional isopleth to be located.

• **Detect isopleth trend** Display on the axes the approximate location of the selected isopleth. Find on each line the location of the selected isopleth (if present) and connect the locations with respect to increasing temperature. See also 3.7. Detect isopleths.



• **Clear isopleth trend** Clear all detected isopleth trends from the axes.

2.7. Wizard Panel



The Wizard Panel allows to calculate successive lines and points at one time, automatically cut the existing lines or run Thermocalc using the Gibbs energy minimization mode.

Mode/Isopleth Wizard

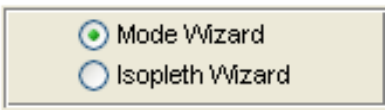
If the **path** of a modal (zero mode) or compositional isopleth line is known, the Wizard Panel allows to calculate the successive lines and points according to a **starting assemblage** and the **successive phases in/out** along the path. See also 3.8. Wizard path calculation.

Cut Wizard

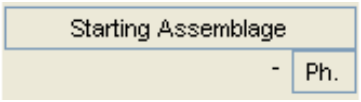
Cut Wizard will try to find the **"begin"** and **"end"** points of each line among the existing points, and will **automatically cut** the line if both the "begin" and "end" points are found. See also 3.8. Wizard path calculation.

Gibbs energy minimization

Run Thermocalc using the Gibbs energy minimization mode (dogmin script) and display on the axes the inferred **stable assemblage** at each calculated point. See also 3.11. Gibbs energy minimization.



• **Mode/Isopleth Wizard** Choose Modal or Compositional isopleth calculation in Wizard mode.
(default - Modal isopleth calculation)



If modal (zero mode) isopleth calculation is selected

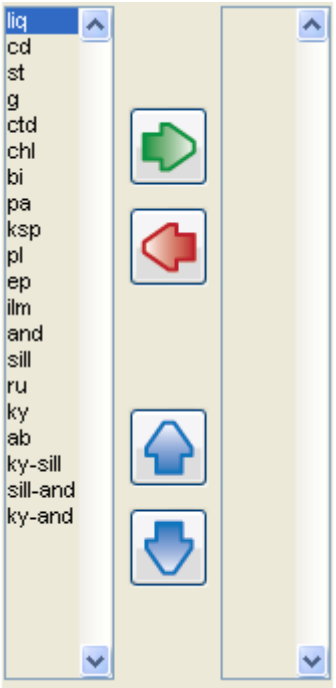
• **Starting Assemblage** Enter the first assemblage of the path that will be calculated, including the phase for which the path is calculated.
(ex: g st pl bi chl)

• **Phase out** Enter name of the phase for which the zero mode path will be calculated.
Note: This phase has to be in the Starting Assemblage.
(ex: st)

If compositional isopleth calculation is selected

• **Name** Enter the name of the compositional isopleth for which the path will be calculated.
(ex: x(st))

• **Value** Enter the value of the compositional isopleth for which the path will be calculated.
(ex: 0.88)



Two listbox menus are used to select the successive phases which appear/disappear along the calculated path.

The first listbox shows all **available phases**, including the possible transitions between the Al_2SiO_5 polymorphs (ky-sill, sill-and or ky-and transitions).

The second listbox (initially empty) has to contain the list of phases which **appear/disappear**, starting from the Starting Assemblage and in the proper order.
Several buttons allow to manage the final list.

• **Add** Add selected phase to the final list.

• **Remove** Remove selected phase from the final list.

• **Move up** Move selected phase up within the final list.

• **Move down** Move selected phase down within the final list.

• **GO** Launch Thermocalc calculation in Wizard mode.

• **Log** Open the log file of the last Wizard calculation run. The log file contains information on the calculated line and points. See also 3.8. Wizard path calculation.

• **Cut Wizard** Cut automatically all existing lines for which the “begin” and/or “end” points have not been specified yet.

• **Do G minimization** Run Thermocalc using Gibbs energy minimization mode. Display three dialog boxes to choose phases, P-T range and P-T calculation step. See also 3.11. Gibbs energy minimization.

3. TUTORIAL

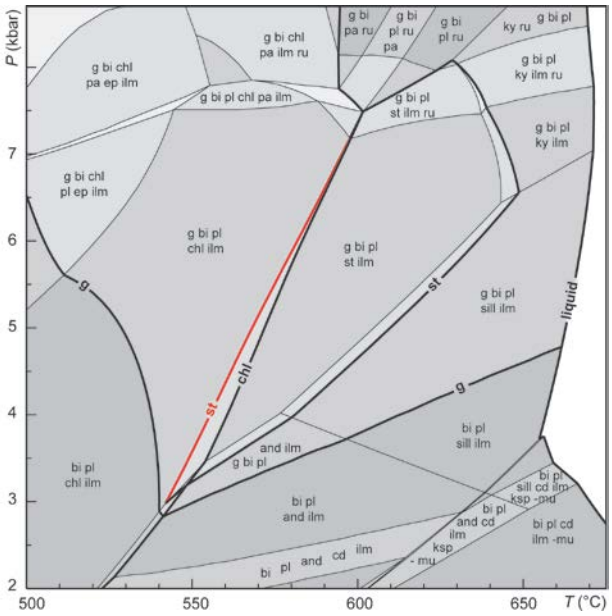
The tutorial uses the demonstration package tc-example. This folder contains:

- Thermocalc run file tc333.exe
- Thermodynamic dataset tc-ds55.txt
- Project file tc-example.txt
- a-x model file tc-MnNCKFMASHTOp&.txt
- Thermocalc preferences tc-prefs.txt
- Drawpd run file dr115.exe
- Drawpd preferences dr-prefs.txt
- Background image example Background_image.jpg
- Saved result file Detect_example.mat

The pseudosection used in this tutorial is a P-T pseudosection calculated for a garnet-staurolite micaschist (sample ES95D) from the Orlica-Śnieżnik Dome (Sudetes). It is described and presented in detail in a contribution by Štípská *et al.* (2012).

3.1. Calculate a zero modal isopleth

In this section, we will calculate a zero modal isopleth line within the P-T pseudosection shown below. It is the staurolite-out line separating the g-bi-pl-chl-ilm and g-bi-pl-chl-ilm-st fields. Note: quartz, muscovite and H_2O are in excess.



P-T pseudosection with the calculated zero modal isopleth highlighted

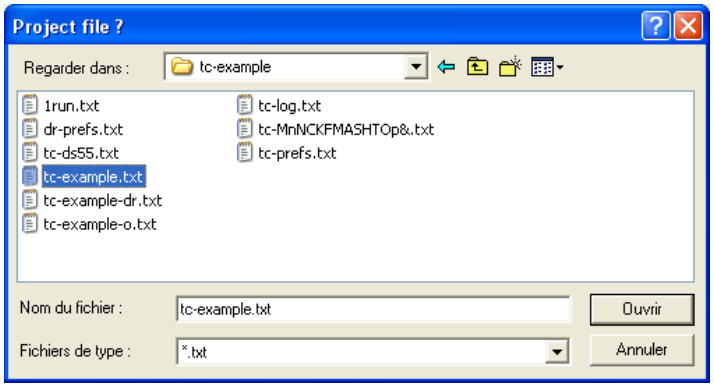
1) Run TCWizard in Matlab

Type *wizz* in the Matlab console or press F5 in the wizz.m file.

➡ The graphical interface opens.

2) Select the project file

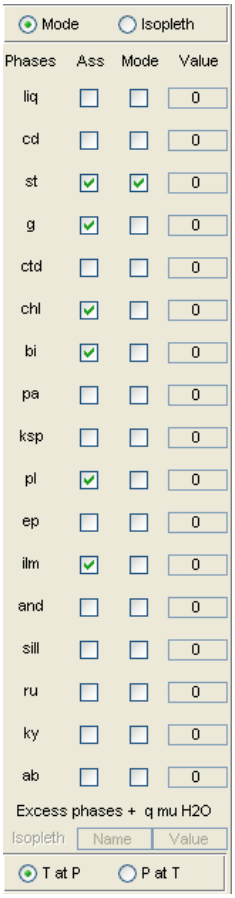
Click the Project File button [Proj. File] , browse to the tc-example folder, and select the **tc-example.txt** file.



➡ The project example is loaded and the list of available phases appears in the Main Calculation Panel.

3) Select Calculation Mode, Assemblage and Phase out

In the Main Calculation Panel, the calculation mode has to be set to Modal isopleth (default) - **Mode**.



We now need to select all phases that are part of the assemblage, including the phase for which the zero modal isopleth will be calculated (in this case, staurolite).

In the column Ass, check the boxes **st, g, chl, bi, pl, ilm**.
In the column Mode, check the box **st**.
In the mode value edit text box for staurolite, type **0** (default).

4) Launch calculation

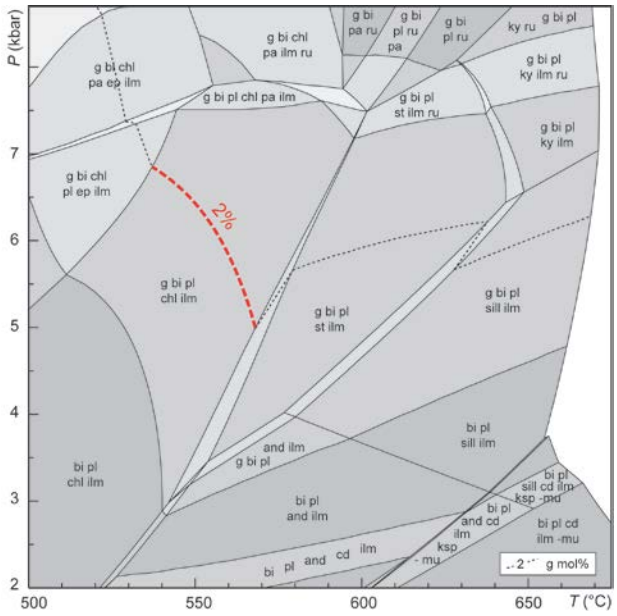
Click the GO button 

.

➡ An hourglass is displayed indicating that the calculation is in progress. When finsihed, the calculated line is displayed in the axes, with the label u1. You can access its data using the data cursor mode (see also 2.5. Information Panel).

3.2. Calculate a non-zero modal isopleth

In this section, we will calculate a non-zero modal isopleth line within the P-T pseudosection shown below. It is the modal isopleth corresponding to 2% of garnet in the g-bi-pl-chl-ilm field. Note: quartz, muscovite and H_2O are in excess.



P-T pseudosection with the calculated non- zero modal isopleth highlighted

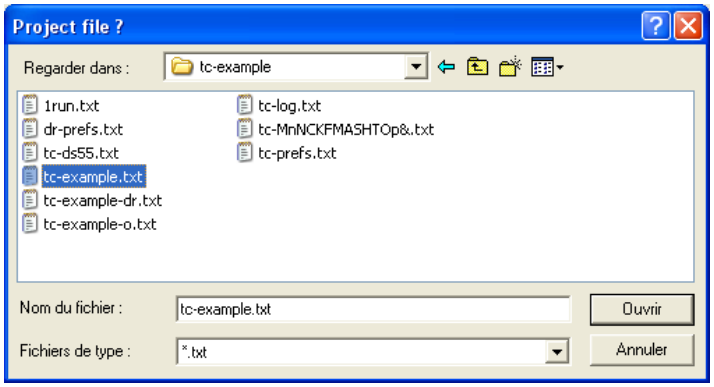
1) Run TCWizard in Matlab

Type *wizz* in the Matlab console or press F5 in the wizz.m file.

➡ The graphical interface opens.

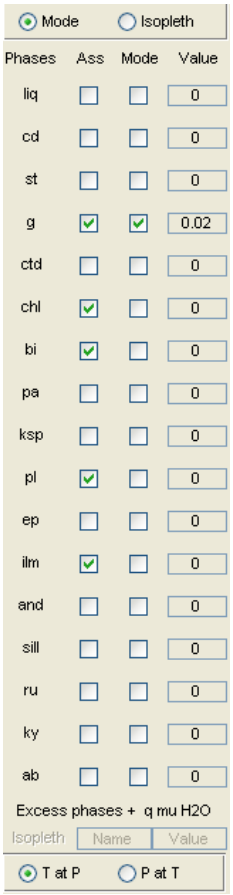
2) Select the project file

Click the Project File button [Proj. File] , browse to the tc-example folder, and select the **tc-example.txt** file.



➡ The project example is loaded and the list of available phases appears in the Main Calculation Panel.

3) Select Calculation Mode, Assemblage and Phase out



In the Main Calculation Panel, the calculation mode has to be set to Modal isopleth (default) - **Mode**.

We now need to select all phases that are part of the assemblage, including the phase for which the non-zero modal isopleth will be calculated (in this case, garnet).

In the column Ass, check the boxes **g, chl, bi, pl, ilm**.
In the column Mode, check the box **g**.
In the mode value edit text box for garnet, type **0.02**.

4) Launch calculation

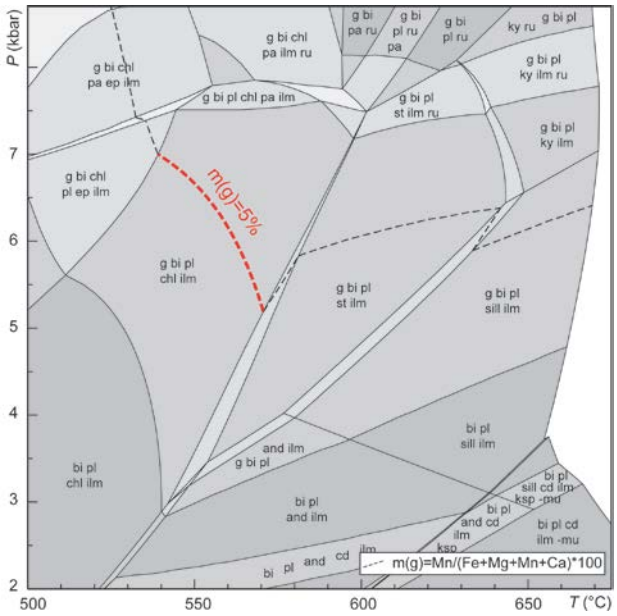
Click the GO button 

.

➡ An hourglass is displayed indicating that the calculation is in progress. When finsihed, the calculated line is displayed in the axes, with the label u1. You can access its data using the data cursor mode (see also 2.5. Information Panel).

3.3. Calculate a compositional isopleth

In this section, we will calculate a compositional isopleth line within the P-T pseudosection shown below. It is the compositional isopleth corresponding to m(g) = 5% in the g-bi-pl-chl-ilm field. Note: quartz, muscovite and H_2O are in excess.



P-T pseudosection with the calculated compositional isopleth highlighted

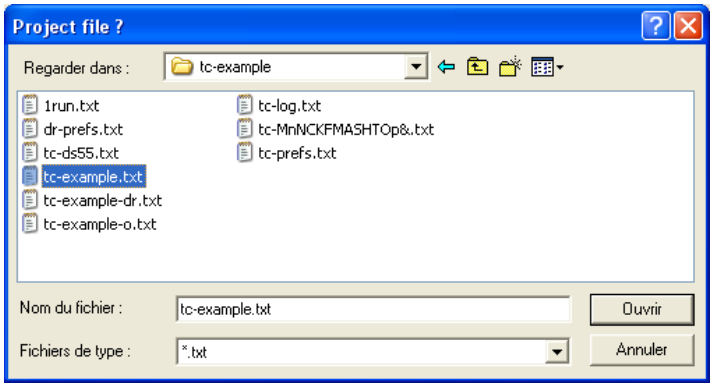
1) Run TCWizard in Matlab

Type *wizz* in the Matlab console or press F5 in the wizz.m file.

➡ The graphical interface opens.

2) Select the project file

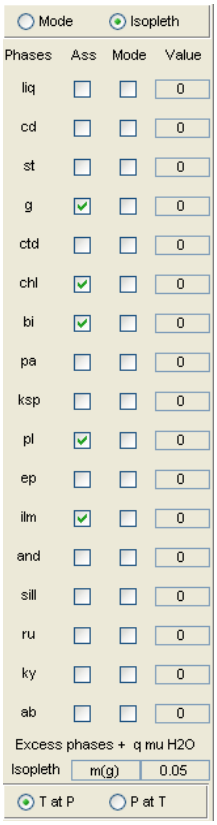
Click the Project File button [Proj. File], browse to the tc-example folder, and select the **tc-example.txt** file.



➡ The project example is loaded and the list of available phases appears in the Main Calculation Panel.

3) Select Calculation Mode, Assemblage, Isopleth name and Isopleth value

In the Main Calculation Panel, the calculation mode has to be set to Compositional isopleth - **Isopleth**.



We now need select all phases that are part of the assemblage

In the column Ass, check the boxes **g, chl, bi, pl, ilm**.
In the Isopleth Name edit text box, type **m(g)**.
In the Isopleth Value edit text box, type **0.05**.

4) Launch calculation

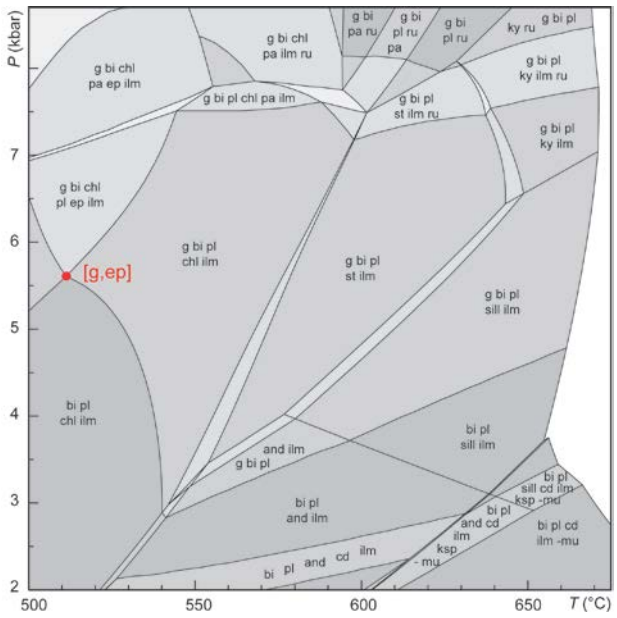
Click the GO button 

.

➡ An hourglass is displayed indicating that the calculation is in progress. When finsihed, the calculated line is displayed in the axes, with the label u1. You can access its data using the data cursor mode (see also 2.5. Information Panel).

3.4. Calculate a point

In this section, we will calculate a point within the P-T pseudosection shown below. It is the point corresponding to zero modal proportions of garnet and epidote, i.e. the intersection between the garnet-out and epidote-out lines. The adjacent fields are g-bi-pl-chl-ilm-ep, bi-pl-chl-ilm-ep, g-bi-pl-chl-ilm, bi-pl-chl-ilm. Note: quartz, muscovite and H_2O are in excess.



P-T pseudosection with the calculated point highlighted

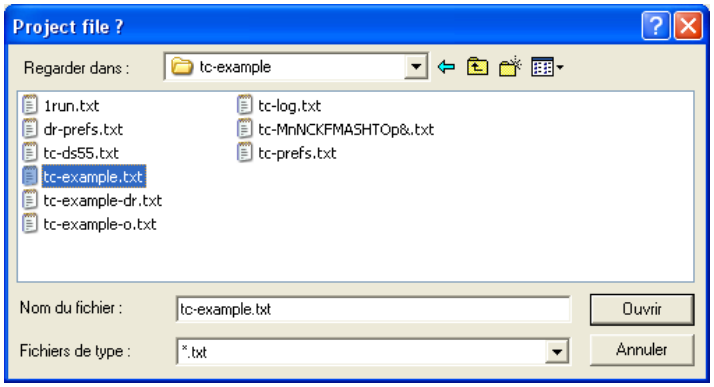
1) Run TCWizard in Matlab

Type *wizz* in the Matlab console or press F5 in the wizz.m file.

➡ The graphical interface opens.

2) Select the project file

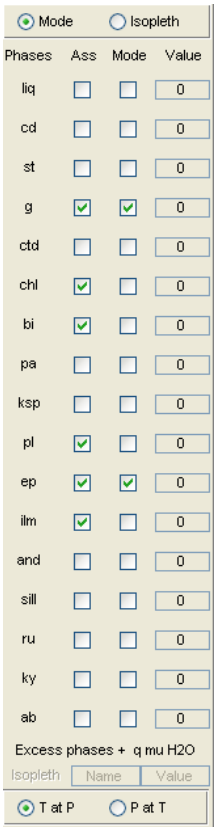
Click the Project File button Proj. File , browse to the tc-example folder, and select the **tc-example.txt** file.



➡ The project example is loaded and the list of available phases appears in the Main Calculation Panel.

3) Select Calculation Mode, Assemblage and Phases out

In the Main Calculation Panel, the calculation mode has to be set to Modal isopleth (default) - **Mode**.



We now need select all phases that are part of the assemblage

In the column Ass, check the boxes **g, chl, bi, pl, ilm, ep**.
In the column Mode, check the boxes **g, ep**.
In the mode value edit text box for garnet and epidote, type **0** (default).

4) Launch calculation

Click the GO button 

.

➡ The calculation is almost immediate. When finished, the calculated point is displayed in the axes, with the label i1. You can access its data using the data cursor mode (see also 2.5. Information Panel).

3.5. Clear a line/point

1) Calculate a line

Following the tutorial 3.1. Calculate a zero modal isopleth, calculate the staurolite-out line between the g-bi-pl-chl-ilm and g-bi-pl-chl-ilm-st fields using the tc-example package.

➡ You should obtain one line labelled u1 in the axes.

2) Calculate a point

Following the tutorial 3.4. Calculate a point, calculate the point corresponding to zero modal proportions of garnet and epidote with adjacent fields g-bi-pl-chl-ilm-ep, bi-pl-chl-ilm-ep, g-bi-pl-chl-ilm, bi-pl-chl-ilm.

➡ You should obtain one point labelled i1 in the axes.

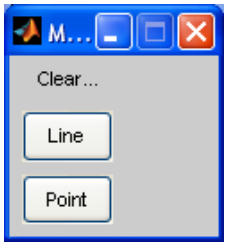
3) Delete a line

If you want to delete an existing line, click the Clear button 

.

➡ A menu will be displayed, with the possibility to choose between :

Clear Line or Clear Point.



Select Line.

➡ A menu with the list of existing lines will appear.

Select the number of the line you want to delete.

! IMPORTANT !

When a line is deleted, all line numbers higher than that of the deleted line are reassigned. They are incremented backwards, so that the line numbers always form a continuous sequence.

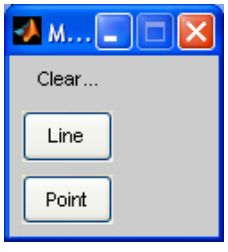
3) Delete a point

If you want to delete an existing point, click the Clear button 

.

➡ A menu will be displayed, with the possibility to choose between :

Clear Line or Clear Point.



Select Point.

➡ A menu with the list of existing points will appear.

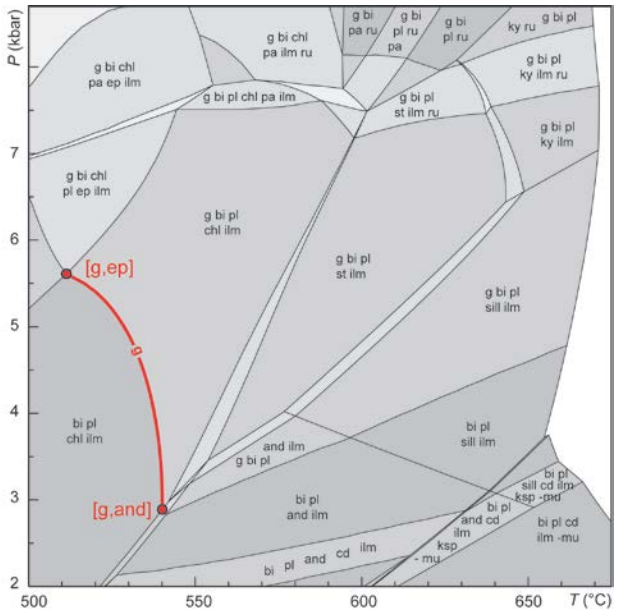
Select the number of the point you want to delete.

! IMPORTANT !

When a point is deleted, all point numbers higher than that of the deleted point are reassigned. They are incremented backwards, so that the point numbers always form a continuous sequence.

3.6. Cut a line

We will now calculate a line and cut it according to its “begin” and “end” points.



P-T pseudosection with the line to be cut highlighted

1) Calculate a line

Following the tutorial 3.1. Calculate a zero modal isopleth, calculate the garnet-out line between the g-bi-pl-chl-ilm and bi-pl-chl-ilm fields using the tc-example package.

➡ You should obtain one line labelled u1 in the axes.

2) Calculate the “begin” and “end” points

Following the tutorial 3.4. Calculate a point, calculate the point corresponding to:

- zero modal proportions of garnet and epidote with the g-bi-pl-chl-ilm-ep assemblage,
- zero modal proportions of garnet and andalusite with the g-bi-pl-chl-ilm-and assemblage.

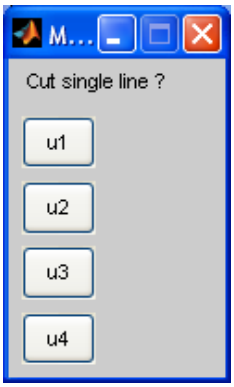
➡ You should obtain two points labelled i1 and i2 in the axes.

You can observe that the line u1 extends farther than the points i1 and i2. In order to get rid of these metastable parts of the line, we will cut u1 according to the “begin” and “end” points.

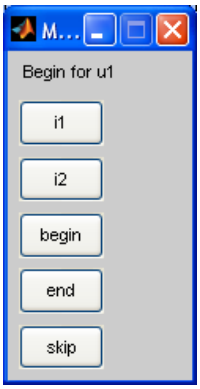
3) Cut the line

Click the **Cut x1**  button.

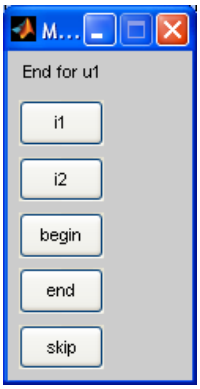
➡Three successive menus will appear.



Menu 1



Menu 2



Menu 3

Menu 1 Display the list of existing lines. Select the line to be cut.

Menu 2 Display the list of existing points and ask for “begin” point.

If the “begin” point is known, select the “begin” point among the list.

If the “begin” point is not defined, select “begin” or “end” (depending on the shape of the curve).

If “skip” is selected, the “begin” point will not be assigned.

Menu 3 Display the list of existing points and ask for “end” point.

If the “end” point is known, select the “end” point among the list.

If the “end” point is not defined, select “begin” or “end” (depending on the shape of the curve).

If “skip” is selected, the “end” point will not be assigned.

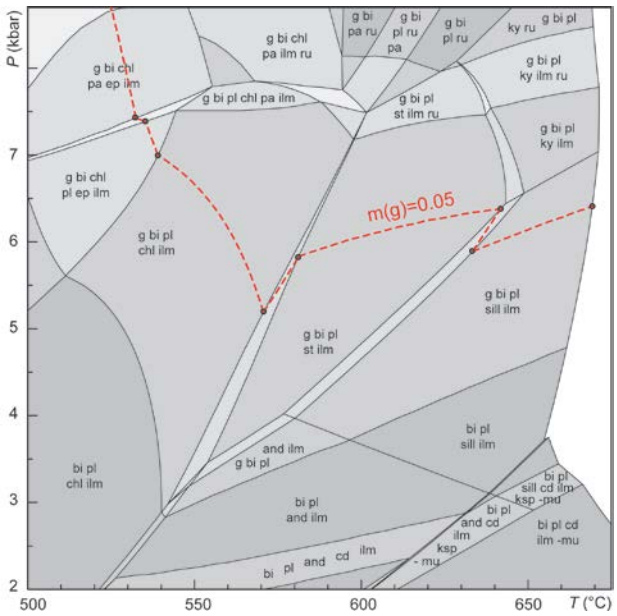
You can also cut successively all existing lines that have not been previously cut using the **Cut xn**  button , and following the same procedure.

Note: If you want to restore the original shape of a line that has been cut, follow the **Cut x1** procedure, but choose skip for both the “begin” and “end” points.

3.7. Detect isopleths

After having calculated several lines or an entire P-T pseudosection, you could be interested in locating the **position of modal or compositional isopleths**. Using the Isopleth Detection Panel, you can overlay the approximate location of isopleths on the existing data.

In the present example, we will try to detect the location of the **garnet compositional isopleth m(g)=0.05** within the pseudosection shown below.



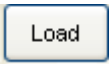
P-T pseudosection with the detected compositional isopleth highlighted

1) Run TCWizard in Matlab

Type *wizz* in the Matlab console or press F5 in the wizz.m file.

➡ The graphical interface opens.

2) Load results

Click the Load button 

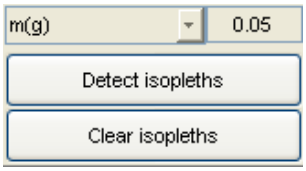
, browse to the tc-example folder, and select the **Detect_example.mat** file.

➡ The results are displayed in the axes.

You can observe the pl-out, pa-out, ep-out, st-out(1), chl-out, sill-out, st-out(2) and liq-out lines that have been previously calculated.

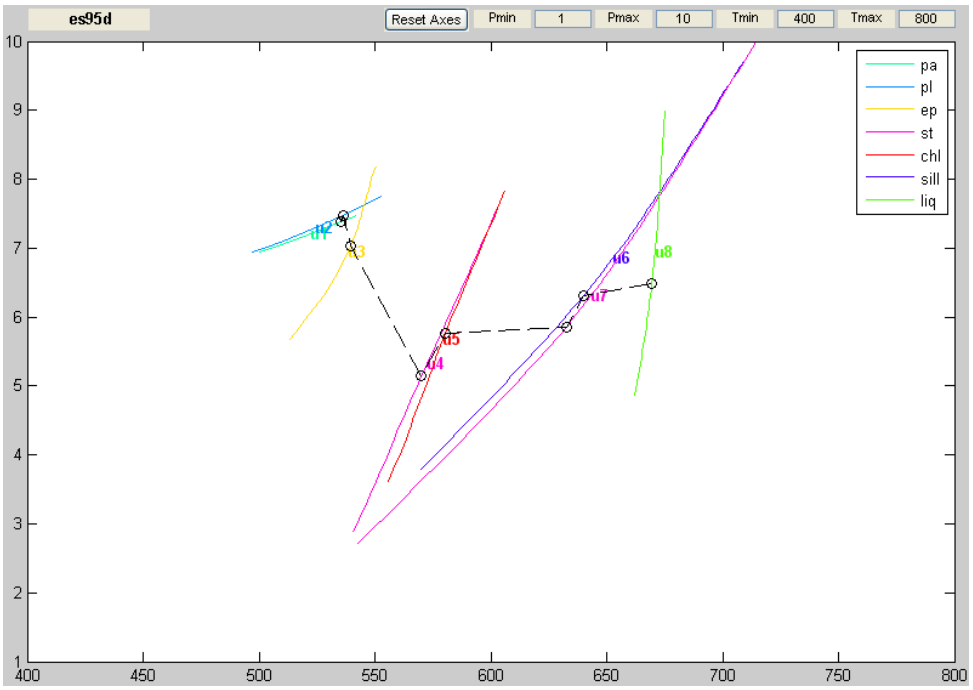
3) Detect isopleths

In the Detect Isopleth Panel, select the **m(g)** compositional isopleth and set the Value to **0.05**



Click the Detect Isoptleths  button.

➡ The results are displayed in the axes.



Results of isopleth detection

The isopleth detection function looks, for each line, if the given value of the selected isopleth is present, i.e. if two points of the line satisfy the condition:

isovalue(Point1) < isovalue(selected) < isovalue(Point2).

The location of the point with the selected isopleth value is then linearly interpolated between the neighbouring points. The different points are finally connected by dotted lines according to increasing temperature.

! Important !

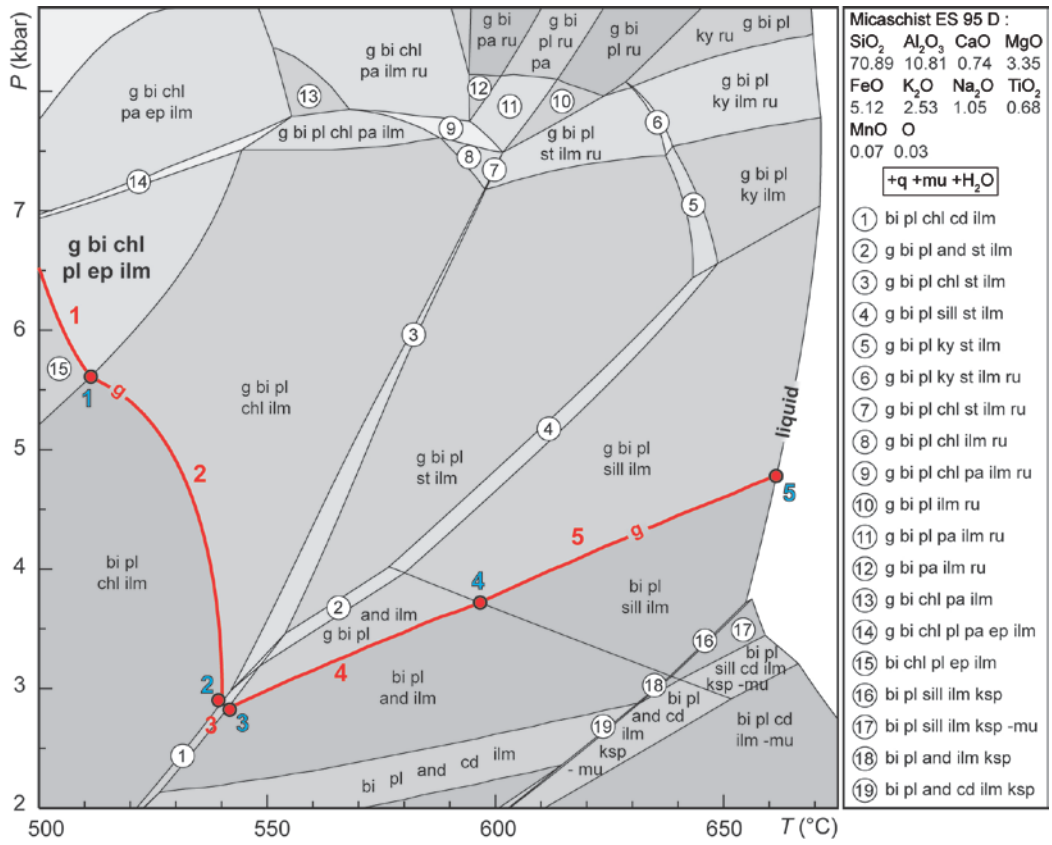
- The Isopleth Detection function can also detect points that lie on metastable parts of the calculated curves.

- The present example illustrates that the connection between points is not always exact and is only informative. The results on the right hand side of the axes show the following connection between dots on: line u5−line u7−line u6. However, the dotted line should connect points located on: line u5−line u6−line u7. It is because the point on line u7 has a lower temperature than the one located on line u6.

3.8. Wizard path calculation

Knowing the topology of a pseudosection or the location of compositional isopleths, you can use the wizard mode to calculate a set of successive line and points. In the present tutorial, we will calculate, from left to right, the garnet-out line in the following pseudosection. The calculation will involve a total of 5 lines and 5 points.

The starting assemblage is g-bi-chl-pl-ep-ilm, and the phase out is g. The garnet-out line successively crosses the lines: epidote-out, andalusite-in, chlorite-out, andalusite-sillimanite transition, liquid-out.



P-T pseudosection with the calculated path highlighted

On the P-T pseudosection, the successive **lines** and **points** will be:

1: g bi pl chl ep ilm - (g)
2: g bi pl chl ilm - (g)
3: g bi pl chl ilm and - (g)
4: g bi pl ilm and - (g)
5: g bi pl ilm sill - (g)

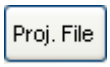
1: g bi pl chl ep ilm - [g, ep]
2: g bi pl chl ilm - [g, and]
3: g bi pl chl ilm and - [g, chl]
4: g bi pl ilm and sill - [g, sill]
5: g bi pl ilm sill liq - [g, liq]

1) Run TCWizard in Matlab

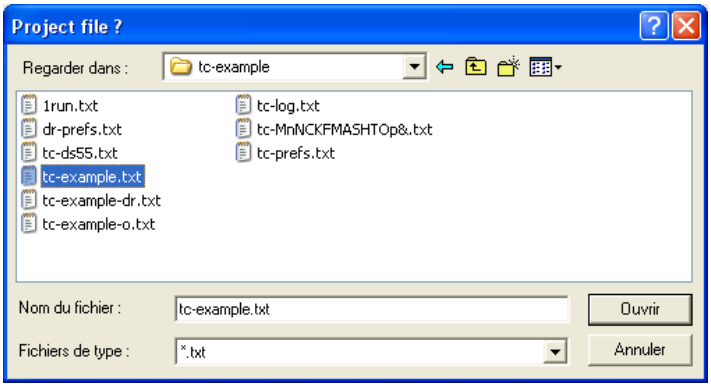
Type *wizz* in the Matlab console or press F5 in the wizz.m file.

➡ The graphical interface opens.

2) Select the project file

Click the Project File button 

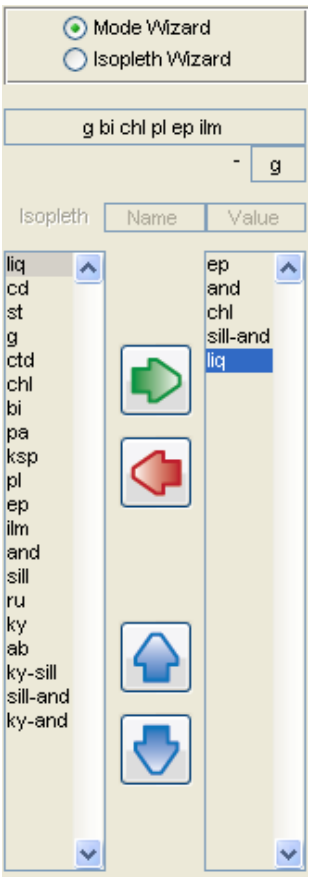
, browse to the tc-example folder, and select the **tc-example.txt** file.



➡ The project example is loaded and the list of available phases appears in the Main Calculation Panel.

3) Wizard calculation parameters

In the Wizard Calculation Panel, the calculation mode has to be set to Modal isopleth (default) - **Mode Wizard**.



We now need to enter the required parameters:

In the Starting Assemblage edit text box, enter **g bi chl pl ep ilm**.

In the Phase out edit text box (-Ph.), enter **g**.

Use the Add/Delete/Move up/Move down buttons to create the list of successive phases. The list in the second listbox should be as follows: **ep, and, chl, sill-and, liq**.

4) Launch calculation

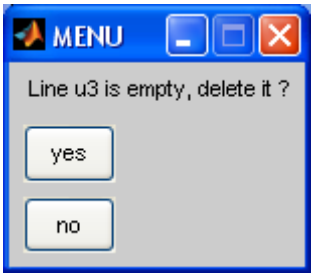
Click the GO button 

.

➡ An hourglass is displayed indicating that the calculation is in progress.

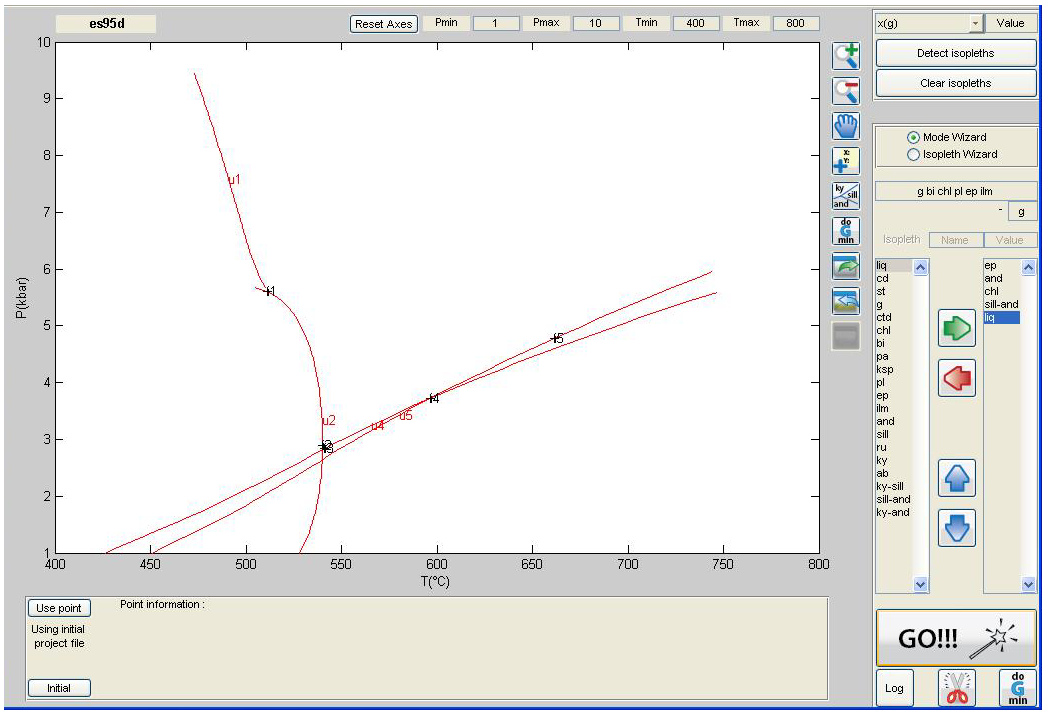
➡ Once the calculation is finished, the program returns 2 successive information messages indicating that lines u3 and u6 were not found.

Line u3 was not found because it is probably too small. We can decide to keep it anyway by clicking **No**.



Line u6 was not found because it lies at suprasolidus conditions. If we do not need that line, we can decide to delete it by clicking **Yes**.

➡ After making these choices, the calculated lines and points are finally displayed in the axes.



Results of Wizard Mode calculation

5) Log file

Any calculation using the wizard mode generates a log file (wizzard_log.txt) in the project directory. You can access it by clicking the 

Log button in the Wizard Panel.

```
Mode wizzard log file

Wizzard calculation parameters
     - starting assemblage : g bi chl pl ep ilm
     - phase out : g
     - path :  -> ep -> and -> chl -> sill-and -> liq
_____________________________________________________________________

RESULTS :

***** Lines *****

-----------------------------------------
Calculated :  bi chl pl ep ilm  - g
Found 43 data points, stored in line u1
-----------------------------------------

-----------------------------------------
Calculated :  bi chl pl ilm  - g
Found 53 data points, stored in line u2
-----------------------------------------

-----------------------------------------
Calculated :  bi chl pl ilm and  - g
Found 0 data points, stored in line u3
-----------------------------------------

-----------------------------------------
Calculated :  bi pl ilm and  - g
Found 52 data points, stored in line u4
-----------------------------------------

-----------------------------------------
Calculated :  bi pl ilm sill  - g
Found 56 data points, stored in line u5
-----------------------------------------

-----------------------------------------
Calculated :  bi pl ilm sill liq  - g
Nothing found, line deleted
-----------------------------------------

***** Points *****

-----------------------------------------
Calculated :  bi chl pl  ilm  - g ep
Found point, stored in point i1
-----------------------------------------
```

```
----------------------------------------
Calculated :  bi chl pl ilm   - g and
Found point, stored in point i2
----------------------------------------

----------------------------------------
Calculated :  bi  pl ilm and  - g chl
Found point, stored in point i3
----------------------------------------

----------------------------------------
Calculated :  bi pl ilm and   - g sill
Found point, stored in point i4
----------------------------------------

----------------------------------------
Calculated :  bi pl ilm sill   - g liq
Found point, stored in point i5
----------------------------------------
```

Overview of the log file

6) Wizard cut

You may then want to cut the calculated lines. For that, you can either use the **Cut x1** or **Cut xn** buttons from the Main Calculation Panel, or the **Cut Wizard** button from the Wizard Panel.

In the present case, we will use the Cut Wizard  button .

Note: The Cut Wizard program can only cut non-empty lines that have both an existing “Begin” and “End” point.

➡ The results of the automatic cut are as follows:

- u1 is not cut because no begin point is defined
- u2 is cut.
- u3 is not cut because it is empty
- u4 is cut
- u5 is not cut. Cut Wizard may not work with lines crossing an Al_2SiO_5 transition.

You can later use the **Cut x1** or **Cut xn** buttons to manually cut u3 and u5 lines.

3.9. Import a background image

You might find useful to display a background image on the axes. It is typically used to spot the location of compositional isopleths in a previously assembled pseudosection.

Note: You can only import a background image after a first calculation has been performed.

1) Calculate a line

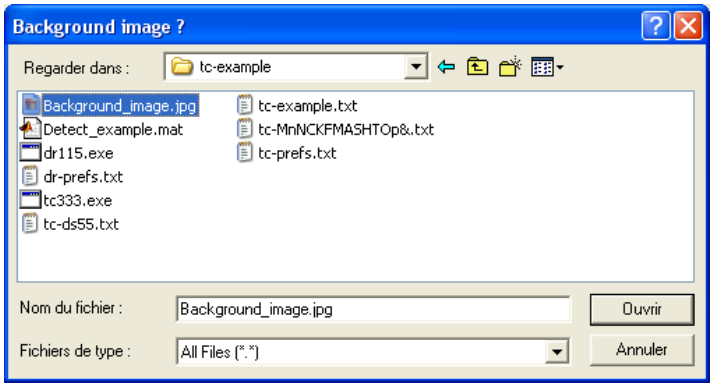
Following the tutorial 3.3. Calculate a compositional isopleth, calculate the compositional isopleth cooresponding to m(g) = 5% in the g-bi-pl-chl-ilm field. (Note: quartz, muscovite and H_2O are in excess). You should obtain one line labelled u1 in the axes.

2) Import background image

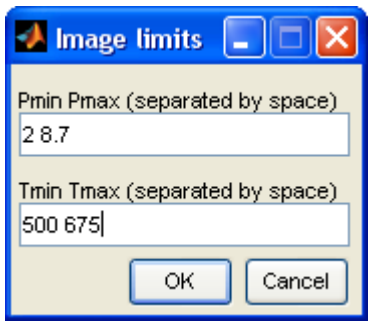
If you now want to see the limits of the line u1, you can import the assembled pseudosection as a background image.

For that, click on the Import Background image  button .

It will display a dialog box to select the image file. Select the "Background_image.jpg" file in the "tc-example" folder.



A dialog box will then ask for the P and T limits of the image.



Enter the following P-T limits:

P: 2 8.7 T: 500 675

➡ The image is displayed if successfully imported.

3) Show/Hide background image

You can decide to show or hide the background image by clicking the Show/Hide  button.

Note: If you save the project, the background image will be saved as well.

Note: The background images have to be Black&White or RGB color images.

3.10. Use new starting guess

In some cases, lines or points are not calculated because the starting values for the compositional isopleths in the a-x model file are too different from those of the calculated object. Using Thermocalc, you have the possibility to set up new starting values that are closer to those of the calculated object. It is possible to do so from the TCWizard interface.

1) Calculate a line

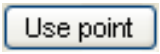
Following the tutorial 3.1. Calculate a zero modal isopleth, calculate the plagioclase-out line between the g-bi-pl-pa-chl-ilm and bi-pa-chl-ilm fields using the tc-example package.
You should obtain one line labelled u1 in the axes.

2) Import a background image

Following the tutorial 3.9. Import a background image, import the "Background_image.jpg" file from the "tc-example" folder. The image limits are P: 2 8.7; T: 500 675.

➡ You will realize that the calculated line u1 corresponds to a metastable part of the plagioclase-out line. This may be because the starting values are too different from those required to calculate the stable part of line u1.

3) Use new starting guess

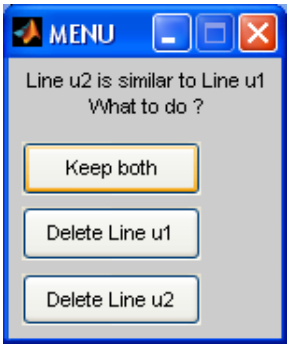
Zoom in to the line u1, enable the Data Cursor  (Axes Tools), and select a point in the left part of u1 (e.g. T=566°C; P=7.84 kbar).
In the Information Panel, click Use Point 

.
➡ The coordinates of the point used for future calculations are now displayed.

4) Re-calculate the line

With the same parameters as in 1), re-calculate the plagioclase-out line between the g-bi-pl-pa-chl-ilm and bi-pa-chl-ilm fields (u1).

➡ A message will tell you that a line with a similar assemblage than that of the line you have just calculated already exists. You can choose to delete of the two lines or to keep both.



In the present case, we would like to compare the results with and without new starting guess. We will therefore choose "**Keep both**".

Note: this message will appear every time the program detects already existing lines after calculation (based on similar assemblage).

The line u2 is displayed in the axes.

You can clearly see that the line u2 is longer than u1, meaning that changing the starting guess helped to calculated the line that appears on the background image.

You can now delete line u1. Keep in mind that the new starting guess will be used until you click the Initial 

button to reset the starting guess back to original.

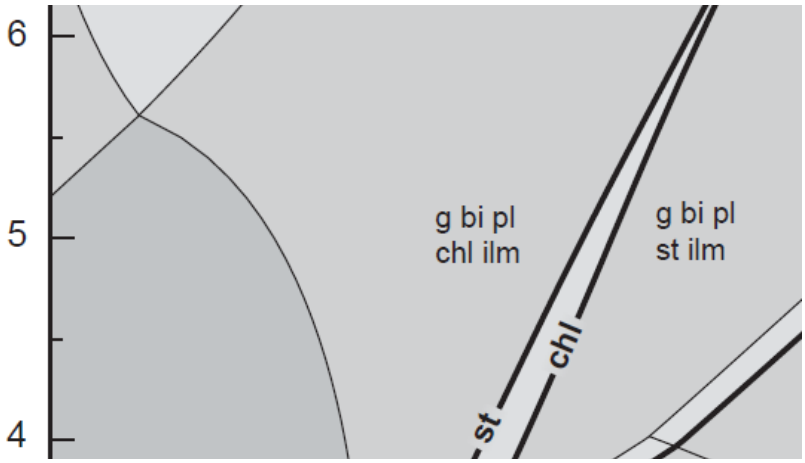
! IMPORTANT !

The use of new starting guess modifies the original project file. However, when closing the TCWizard figure, a special function restores the original project. You should be aware that, if TCWizard is not closed normally, new starting guess may stay in the original project file.

3.11. Gibbs energy minimization

You may wish to know which assemblage is stable in a given P-T region of the calculated pseudosection. For that, you can use the Gibbs energy minimization mode available in Thermocalc, via the TCWizard interface.

In this example, we will focus on the region enlarged below. There, the st-out and chl-out lines lie close to each other, i.e. it looks like the g-bi-pl-chl-ilm assemblage changes to the g-bi-pl-st-ilm assemblage. We will examine the stable assemblages around 5 kbar and between 560-580°C.



Enlarged part of the P-T pseudosection at 4-6 kbar/500-600°C

1) Run TCWizard in Matlab

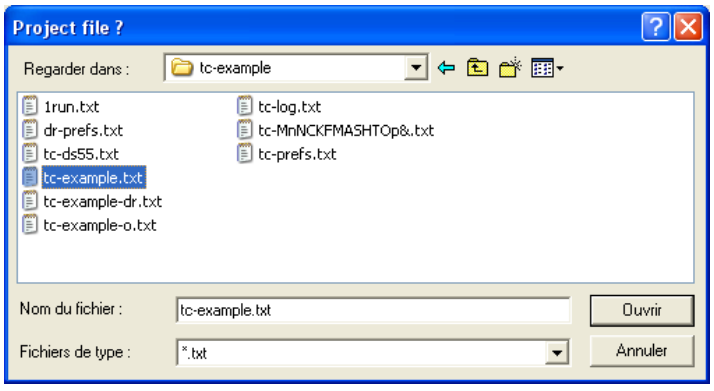
Type *wizz* in the Matlab console or press F5 in the wizz.m file.

➡ The graphical interface opens.

2) Select the project file

Click the Project File button 

, browse to the tc-example folder, and select the **tc-example.txt** file.



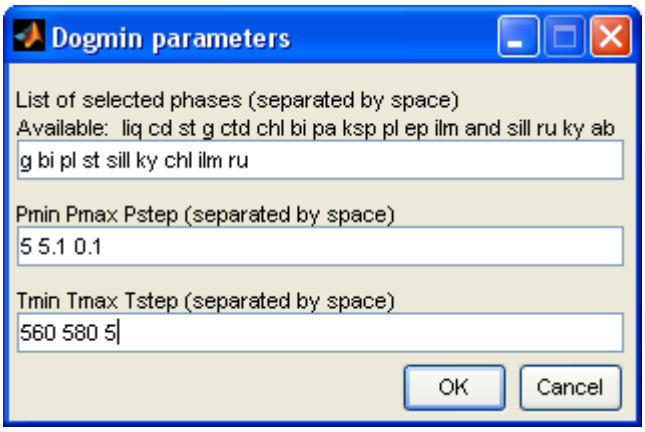
➡ The project example is loaded and the list of available phases appears in the Main Calculation Panel.

3) Run Thermocalc with Gibbs energy minimization mode (dogmin)

Click the Dogmin button 

.

➡ A dialog box with three different questions will appear



Question 1 *List of possibly stable phases*

Enter the phases you would like to test the stability of. A list of all available phases is shown for help.

Enter: g bi pl st sill ky chl ilm ru

Note: Excess phases are automatically included in the calculations.

Question 2 *P range and step*

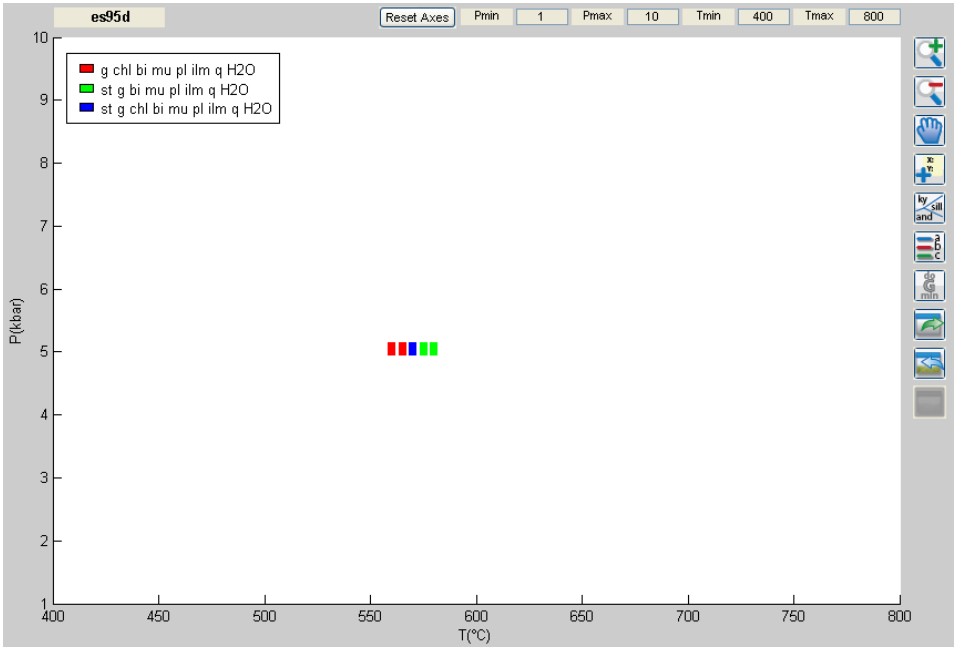
Enter Pmin, Pmax and Pstep of the calculation.

Enter: 5 5.1 0.1

Question 3 *T range and step*

Enter Tmin, Tmax and Tstep of the calculation.

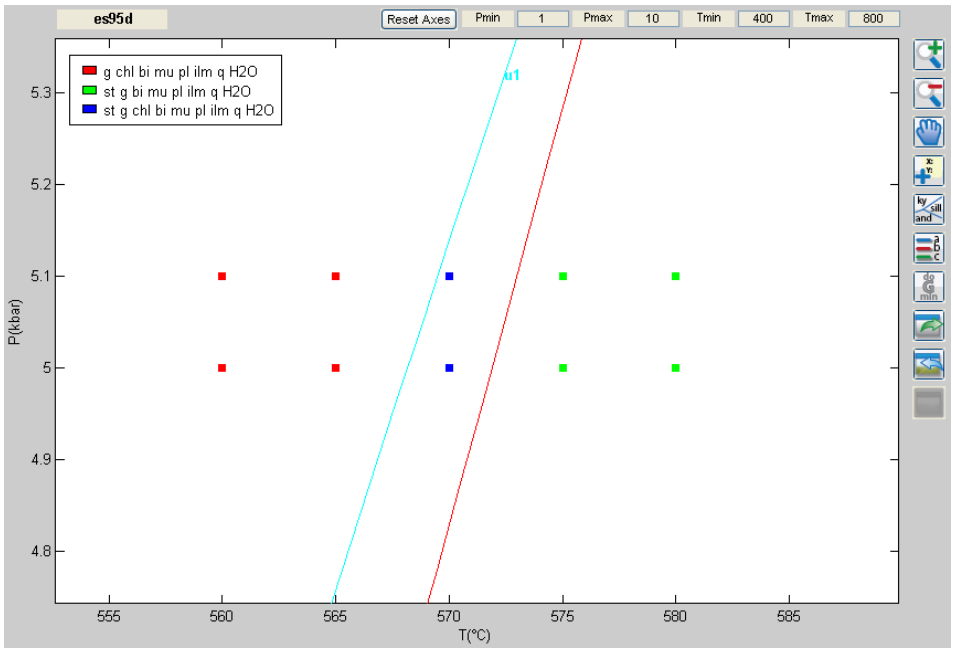
Enter: 560 580 5



Results of Gibbs energy minimization calculation

The Gibbs energy minimazation calculation finds the assemblage with the lowest Gibbs free energy at the selected P-T conditions. The results are displayed as squares with different colours according to the different assemblages.

Following these results and the tutorial 3.1. Calculate a zero modal isopleth, you can now calculate the staurolite-out and chlorite-out lines using the assemblage g st bi chl ilm pl. When zooming in the region ~ 5 kbar/560-580°C, you should see the following results.



Enlarged view of Gibbs energy minimization calculation results (with additional lines)

Note: Dogmin calculations are performed along isobaric sections (rows) with varying temperature. In the case of the example, it calculates 2 rows at 5 and 5.1 kbar, and at T=560, 565, 570, 575, 580°C.

Note: The maximum variance to be looked at is set to 6 (default). You can change it manually, at your own risk, in the dogmin_wizzard.m file at line 113.

4. MATLAB® FILES AND PROGRAM

4.1. TCWizard package

List of files in the TCWizard package

Matlab® functions (.m files)

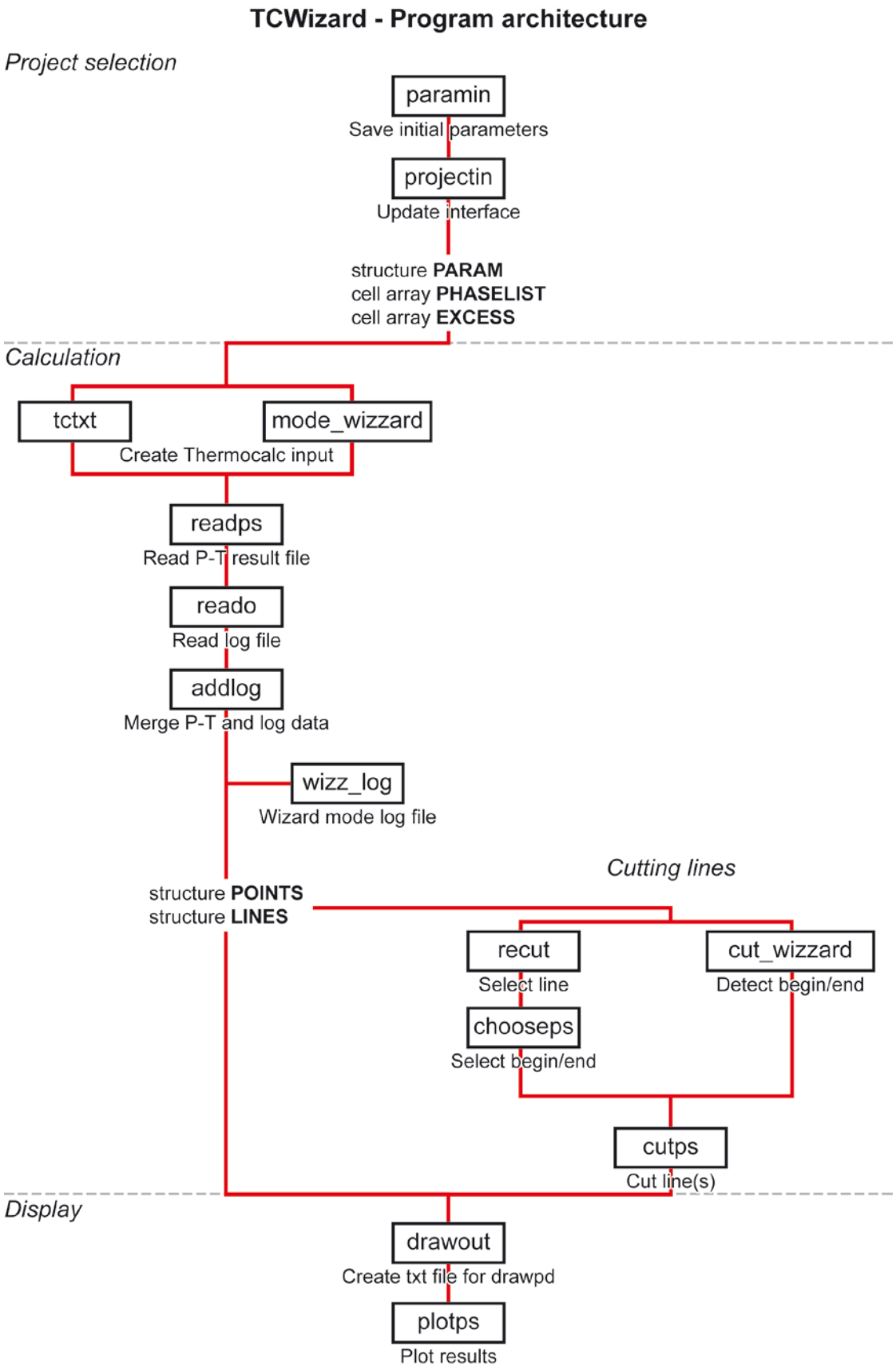
addlog.m	Add log data to line/point structures
al2sio5.m	Show/Hide Al2SiO5 orientation diagram
bcgim.m	Show/Hide background image
bcgim_in.m	Import background image and parameters
buttonadd.m	Add selected phase in the phase list for the Wizard mode
buttondel.m	Delete selected phase in the phase list for the Wizard mode
buttondown.m	Move down selected phase in the phase list for the Wizard mode
buttonup.m	Move up selected phase in the phase list for the Wizard mode
chooseps.m	Ask for line limits (begin and end) and update line structure
clearlast.m	Delete selected line or point
cursorupdate.m	Update function for the properties of the point selected with the cursor
cutps.m	Cut lines according to user's selected limits
cut_wizzard.m	Automatically detect begin and end points for lines
datacur_on.m	Turn on the datacursor mode and turn off all other modes
detect.m	Detect location of user's selected isopeth value on the available lines
dogmin_disp.m	Show/Hide dogmin results
dogmin_plot.m	Plot results of Gibbs energy minimization mode (dogmin)
dogmin_wizzard.m	Run Thermocalc with Gibbs energy minimization mode (dogmin)
drawout.m	Create dr-out.txt file with results for drawpd (in the project directory)
loadpl.m	Load matlab .mat file with initial parameters previous data
mode_wizzard.m	Calculate data using Wizard mode
pan_on.m	Turn on the pan mode and turns off all other modes
paramin.m	Gather initial parameters for Thermocalc calculations
plotps.m	Plot Thermocalc results
projectin.m	Add available phases to the main figure
radioupdate1.m	Enable/disable text boxes for "Isopleth" or "Mode" mode
radioupdate2.m	Enable/disable text boxes for "Mode " or "Isopleth" Wizard mode

reado.m	Read Thermocalc results from the tc-log.txt file
readps.m	Read Thermocalc results from the tc-xxx-dr.txt file
recut.m	Clear existing limits of selected line to allow subsequent cutting
resetaxes.m	Reset axes to P-T limits from the project file
savefig.m	Export axes into eps file
savepl.m	Save the initial parameters and data calculated in a matlab .mat file
sizeupdate.m	Update function for resizing the main window
tckiller.m	Kill Thermocalc running in the background if error
tctxt.m	Create the temporary text file to run Thermocalc
textguess_off.m	Restore the original project file
textguess_on.m	Add selected starting guesses to the project file
wizz.m	Main program to be executed
wizz_log.m	Generate log file of Wizard mode calculation
zoom_in.m	Turn on the zoom mode (positive) and turns off all other modes
zoom_out.m	Turn on the zoom mode (negative) and turns off all other modes

Icons (.png files)

button_add.png	button_dogmin.png	button_pan.png
button_alsioff.png	button_dogminoff.png	button_sablier.png
button_alsion.png	button_dogminon.png	button_savefig.png
button_cut1.png	button_down.png	button_up.png
button_cutn.png	button_gowiz.png	button_zoomin.png
button_cutw.png	button_imhide.png	button_zoomout.png
button_datacur.png	button_importim.png	
button_del.png	button_imshow.png	

4.2. Program architecture



4.3. Important variables

Project selection

param structure with intitial parameters

- pathin = path to the Thermocalc package
- project = project name (tc-*projectname*.txt)
- resultfile = name of the result file (tc-*projectname*-dr.txt)
- axfile = a-x model file (ex: tc-NCKFMASH)
- ofile = name of the detailed result file (tc-*projectname*-o.txt)
- PTrange = user's selected P&T min, max (in the project file)
- matpath = path to the TCWizard Matlab® package
- protext = character array containing the entire project file

phaselist cell array of available phases for calculation (withouth excess phases)

excess cell array of excess phases specified in the project file

iminfo structure with parameters of the background image

- P = Pmin and Pmax of the image
- T = Tmin and Tmax of the image
- path = path to the image file

Calculation

lines structure with calculated lines

- lnum = line number (ex: u1)
- lass = assemblage (ex: g st pl - chl)
- lal = assemblage list (ex: p1 = g, p2 = st ...)
- lcrd = P-T coordinates (ex: 1.5 550.0)
- lphase = phase out
- lbegin = coordinates of begin point
- ltbegin = name of begin point
- lend = coordinates of end point
- ltend = name of end point
- linef = P-T coordinates after cutting

- liso = modal or compositional isopleth, if present (ex: x(g)=0.95)
- keep = marker to keep line (0=asking if delete 1=not asking if delete)
- sim = marker if similar object (0=unique 1=similar)
- … = additional fields with compositional isopleth and mode data

points structure with calculated points

- pnum = point number (ex: i1)
- pass = assemblage (ex: g st pl - bi chl)
- pal = assemblage list (ex: p1 = 'g', p2 = 'st' ...)
- pcrd = P-T coordinates (ex: 1.5 550.0)
- pphase1 = phase out 1
- pphase2 = phase out 2
- piso1 = isopleth 1 value (ex: x(g)=0.95)
- piso1 = isopleth 2 value (ex: g=0.01)
- sim = marker if similar object (0=unique 1=similar)
- … = additional fields with compositional isopleth and mode data

data structure with Gibbs energy minimazation results (dogmin)

- P = P coordinate
- T = T coordinate
- ass = point assemblage
- color = color code

5. TROUBLESHOOTING

The present section lists the known problems that might be encountered during the use of TCWizard.

• tc333.exe still running in the background

Although safety conditions are set in the programs, an erroneous input in the Main Calculation Panel or the Wizard Panel may cause the calculations not to end properly. This will result in no data being displayed. However, one must pay attention to the fact that tc333.exe (launched by Matlab for calculation) might still be running in the background. In that case, one will have to terminate this process using the task manager (Terminate process tc333.exe).

• Altered project file

The use of the Gibbs energy minimization mode (dogmin) modifies the initial project file, and restores it at the end of the calculation. If, for any reason, the dogmin calculation does not end properly, the initial project file will not be restored. However, a special function restores the initial project file when the main TCWizard interface is closed.

For the next use of TCWizard, it is still important to make sure that the project file is not altered.

• Point information not displayed

It can happen that Thermocalc does not write the mode information in the log file. In that case, the Information Panel will remain empty if a point belonging to that line is selected.

6. LINKS & REFERENCES

TCWizard webpage:

http://eost.unistra.fr/recherche/ipgs/dylbas/dylbas-perso/benoit-petri/software1/

Thermocalc webpage:

http://www.metamorph.geo.uni-mainz.de/thermocalc/

PyPSbuilder (software by O. Lexa):

http://petrol.natur.cuni.cz/~ondro/pypsbuilder:download

Powell R., Holland T. & Worley B., 1998. Calculating phase diagrams involving solid solutions via non-linear equations, with examples using THERMOCALC. *Journal of Metamorphic Geology*, 16, 577–588.

Štípská P., Chopin F., Skrzypek E., Schulmann K., Pitra P., Lexa O., Martelat J-E., Bollinger C., Žáčková E., 2012. The juxtaposition of eclogite and mid-crustal rocks in the Orlica-Śnieżnik Dome, Bohemian Massif. *Journal of Metamorphic Geology*, 30, 213-234.

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