

Introduction to phase diagram calculations in KFMASH – tutorial III

by Simon Schorn (October 27, 2021)

This is the third and last of three tutorials, designed to give you a brief introduction to phase diagram calculations using THERMOCALC. Here we look into pseudosections. This tutorial follows up on the previous lessons dealing with P – T projections and AFM compatibility diagrams in the simplified metapelite system of K_2O – FeO – MgO – Al_2O_3 – SiO_2 – H_2O (KFMASH). I suggest to complete these tutorials in the right order, but this is not strictly required. Before diving into calculations, I recommend you go through the “get started” section of the website and documentation, in particular “[Phase diagram introduction](#)”. Also it is a good idea to read some of the key papers, in particular [Powell *et al.* 1998](#) (Calculating phase diagrams involving solid solutions via non-linear equations, with examples using THERMOCALC. *J Metam Geol*, 16(4), 577–588).

This tutorial was made using THERMOCALC v3.50beta (version from 16.01.2020) and drawpd v1.18 (see THERMOCALC [download guide](#) and [downloads](#) on the webpage) on a Windows machine.

In your THERMOCALC-folder you should have the following files:

tc350	THERMOCALC executable
tc-prefs	THERMOCALC preferences file
tc-pseudotute	script file
tc-ds62	thermodynamic dataset
tc-mp50KFMASH	activity–composition file

I like to keep everything related to the drawfile in a separate folder, but this is optional. The “draw”-folder should contain the following files:

dr118	drawpd executable
dr-prefs	drawpd preferences file
dr-project	empty draw file

The complete draw-file for the P – T projection is "dr-kfmash-grid" and the edited result is the pdf-file "KFMASH-grid".

The file tc-prefs contains the following:

```
dataset      62                % which thermodynamic dataset file to use
scriptfile   pseudotute        % which scriptfile to use
calcmode     1                 % what sort of calculation to do
```

for THERMOCALC to automatically use this script file, and specifying you are doing phase diagram calculations. The script "calcmode 1" specifies that you are doing phase diagram calculations.

KFMASH P – T pseudosection

A P – T *pseudosection* shows the predicted equilibrium mineral & fluid assemblages (including modes and compositions) for a particular bulk composition. 'Section' in this context means a 2-dimensional 'cut' through the *total phase diagram* – which contains *all* information on phase equilibria in $c^1 + 1$ dimensions – with respect to the chosen bulk composition. We do this because a total phase diagram is an n -dimensional body that cannot be graphically represented. The 'pseudo' comes in because the mineral compositions lie outside the section (they are different from the bulk rock composition), making a pseudosection a multi-dimensional version of a pseudo-binary phase diagram.

The pseudosection presented in this tutorial is calculated for an amphibolite-facies garnet–kyanite micaschist from the Eastern Alps from [Schorn, 2018](#) (Dehydration of metapelites during high- P metamorphism: The coupling between fluid sources and fluid sinks. *J Metam Geol*, 36(3), 369–391). To adapt the whole rock composition I simply stripped it from all non-KFMASH components, which is a simplification², but acceptable for our purposes.

¹ c is the number of components in the system

²By ignoring Na₂O and CaO the Al₂O₃ stored in plagioclase stays behind, and the total alumina-content is slightly overestimated.

I will start with the staurolite isograd, like in the two previous tutorials. It is given by the coexistence of garnet and chlorite reacting to staurolite and biotite, or written using THERMOCALC phase abbreviations:



where again we assume that muscovite, quartz and H₂O are always present (*in excess*).

Before starting THERMOCALC, we'll have quick look at some important scripts in the scriptfile ("tc-pseudotute.txt"). There is a number of scripts available for different types of calculations (see the documentation on the website for more), but here the most important lines are

```
axfile mp50KFMASH          % mandatory script
diagramPT 0.1 18 440 720    % minP maxP minT maxT; mandatory script
pseudosection yes          % mandatory script
```

The axfile script tells THERMOCALC which axfile to use; diagramPT gives the *PT* (in kbar, °C) of the phase diagram being drawn (plus a little bit); and "pseudosection yes" says that we are doing a pseudosection calculation. The script "with someof" is followed by a list of all the phases that might occur in the diagram – it means we can focus on the relevant phases, not the whole list of phases in the axfile, which can be very long. Note that the "with someof" list includes phases that are in excess, even though these are specified in a separate (non-mandatory) script: "inexcess mu q H₂O".

Alright, let's fire up THERMOCALC!

When executing the program, you will see in the terminal window³:

```
THERMOCALC 3.50 (Free Pascal version)
```

```
the summary output is in the file, "tc-pseudotute-o.txt"
```

```
other (eg drawpd) output is in the file, "tc-pseudotute-dr.txt"
```

³as the scripts and the output are still evolving, the words on screen may be a bit different from what is indicated in the text here

```
more csv format in the file, "tc-pseudotute2.csv"
```

[illegible]

THERMOCALC 3.50 running at 13.48 on Thu 21 Oct,2021
using tc-ds62.txt produced at 20.08 on Mon 6 Feb,2012
with axfile tc-mp50KFMASH.txt and scriptfile tc-pseudotute.txt

reading ax: q liq mu bi opx sa cd st chl ctd spl ksp sill and ky q H2O

```
with someof: g liq mu bi opx cd st chl ctd spl ksp sill and ky q H2O (from sc#
inexcess: mu q H2O - auto included (from script)
choose phases :
```

This is where you will need to specify the phases that are taking part in the reaction we are trying to calculate. Note that as specified in the scriptfile, we want to set quartz (q), muscovite (mu) and H₂O in excess. Make sure that the phases which should be in excess are specified following the "inexcess" keyword.

So, next we type the other phases involved in the staurolite isograd, followed by the return key⁴:

⁴User-input is highlighted in red and comments in blue

choose phases : g chl st bi <return>

fluid is just H2O

in excess: mu q H2O

specification of xyz starting guesses of phases

in the scriptfile: g mu bi st chl; not in the scriptfile: none

specification of overall PT window:

overall PT window is P: 0.1 to 18.0 kbar, and T: 440 to 720°C (from script)

variance of required equilibrium (1?) : <return>

specification of mode isopleths

you may set zero modal proportions, from: g mu bi st chl q H2O

which to set : <return> (not setting any phase to 0)

no modes set

original variance = 1, effective variance = 1 (0, 0)

calculate T at P (rather than P at T) ? <return>

specification of PT calcs:

P at which T of reactions to be calculated

P calcs: between P(low) and P(high), with P increment : 5 15 0.1 <return> (inspecting a large P window at steps of 0

which phases : g chl st bi <return>
 variance of required equilibrium (1?) : <return>
 you may set zero modal proportions, from: g mu bi st chl q H2O
 which to set : <return> (not setting any phase to 0)
 calculate T at P (rather than P at T) ? <return>

specification of PT window:

P range over which T of reactions to be calculated

P window: P low,high : 5 15 <return> (inspecting a large P window)

T window within which reactions expected to lie

T window: T low,high : 500 700 <return> (inspecting a large T window)

use the P interval in the datafile script ? <return> (using the interval set in the scriptfile)

We get:

using overall T window for the T window within which reactions expected to lie

P interval = 0.1 kbar (from script)

specification of bulk composition

composition (from bulk script)

H2O	SiO2	Al2O3	MgO	FeO	K2O
17.215	57.867	12.980	3.176	6.430	2.333

<=====>

phases: g bi st chl (mu, q, fluid)

221 <note this>

```
-----
P (kbar)      T (°C)      x (g)      x (mu)      y (mu)      x (bi)      y (bi)      Q (bi)
    5.300      532.82      0.9960      0.9659      0.9440      0.9875      0.2149      0.004015
                x (st)      x (chl)      y (chl)      QAl (chl)      Q1 (chl)      Q4 (chl)
                0.9955      0.9823      0.7833      0.2165      0.01011      0.02727
```

30g + 46mu + 17chl = 46bi + 10st + 69q + 48H2O

```
-----
P (kbar)      T (°C)      x (g)      x (mu)      y (mu)      x (bi)      y (bi)      Q (bi)
    5.400      535.31      0.9907      0.9239      0.9417      0.9705      0.2162      0.009502
                x (st)      x (chl)      y (chl)      QAl (chl)      Q1 (chl)      Q4 (chl)
                0.9894      0.9584      0.7782      0.2216      0.02229      0.05762
```

30g + 46mu + 17chl = 46bi + 10st + 69q + 49H2O

```
-----
...
```

The output contains the input values for pressure that we have chosen, and the corresponding temperature where THERMOCALC has calculated the staurolite isograd to be stable. The other parameters such as x(g), y(bi), Q(chl) and so on describe the calculated composition of the participating mineral phases. Additionally, THERMOCALC gives us the reaction that is involved in the equilibrium we calculated – which is indeed the staurolite isograd.

Notice that even though we have asked to calculate the reaction starting at 5 kbar, THERMOCALC has only found values above 5.25 kbar, and produces a string of 221 beforehand. These typically flag that it has tried to find solutions for $P = 5.0\text{--}5.2$ kbar, but the reaction terminated in a subsystem,

implying that one or several of the participating phases assumed an end-member composition.

This type of output is identical to what we have calculated in the P – T projection tutorial. If you scroll down the THERMOCALC output, at about 7.25 kbar & 576 °C you'll find:

```
...
-----
P (kbar)      T (°C)      x (g)      x (mu)      y (mu)      x (bi)      y (bi)      Q (bi)
    7.200      575.12      0.9015      0.5584      0.9075      0.6975      0.2282      0.09601
              x (st)      x (chl)      y (chl)      QAl (chl)      Q1 (chl)      Q4 (chl)
              0.8766      0.6060      0.6974      0.3024      0.07896      0.1256

27g + 51mu + 21chl = 51bi + 10st + 76q + 62H2O

mode          g          mu          bi          st          chl          q          H2O      #
              0.2919      0.01858      0.1334      0.1578      0.3417      0.05658      -#
    0.008991      0.3097              0.1198      0.1702      0.3379      0.05346      -#
-----
...
```

Beginning at 7.20 kbar, THERMOCALC now also plots the modal amounts of the participating phases as well as reaction 1. This means that this section of the staurolite isograd is both stable and 'seen' by the chosen bulk composition, whereas the portion where no modes are calculated is not expressed in this bulk composition. The reaction is still stable, though!

Notice that the modes for garnet and biotite are only given on one side of the reaction. This indicates that the assemblage on one side of the reaction is biotite–staurolite–chlorite and garnet–staurolite–chlorite on the other (both +q +mu +H₂O). Also, the modes of both garnet and biotite tend towards 0 down pressure. This tells us that in this bulk composition, the staurolite isograd terminates at low pressure in an invariant point where the modes of

garnet and biotite both are equal to 0.

When scrolling down the THERMOCALC out put you'll note that some phases change sides in the mode output:

...

```
-----
P (kbar)      T (°C)      x (g)      x (mu)      y (mu)      x (bi)      y (bi)      Q (bi)
      8.100      591.62      0.8595      0.4764      0.8932      0.5899      0.2276      0.1216
              x (st)      x (chl)      y (chl)      QAl (chl)      Q1 (chl)      Q4 (chl)
              0.8165      0.4883      0.6666      0.3332      0.07235      0.09090
```

25g + 53mu + 22chl = 53bi + 10st + 78q + 70H2O

mode	g	mu	bi	st	chl	q	H2O	#
	9.626e-5	0.1702	0.1461	0.2255		0.3557	0.1024	-#
	0.06365	0.3097		0.1225	0.1021	0.3262	0.07597	-#

...

This suggests that the staurolite isograd actually separates three divariant fields, with the third having the assemblage garnet–staurolite–biotite (+q +mu +H₂O).

We now calculate the point at low pressure by simply setting both garnet and biotite to 0. Hit return in THERMOCALC if you didn't close the window, or start it again:

last time was: g bi st chl + mu q H2O

choose phases : <return> (same phases as before)

fluid is just H2O
in excess: mu q H2O

specification of xyz starting guesses of phases
in the scriptfile: g mu bi st chl; not in the scriptfile: none

specification of overall PT window:
overall PT window is P: 0.1 to 18.0 kbar, and T: 440 to 720°C (from script)
variance of required equilibrium (1?) : <return>

specification of mode isopleths
you may set zero modal proportions, from: g mu bi st chl q H2O
which to set : g bi <return> (here we set g & bi to 0)

specification of bulk composition
composition (from bulk script)

H2O	SiO2	Al2O3	MgO	FeO	K2O
17.215	57.867	12.980	3.176	6.430	2.333

<=====>

phases: g bi st chl (mu, q, fluid)

P (kbar)	T (°C)	x (g)	x (mu)	y (mu)	x (bi)	y (bi)	Q (bi)
----------	--------	-------	--------	--------	--------	--------	--------

7.101	573.18	0.9061	0.5695	0.9092	0.7105	0.2280	0.09235
		x(st)	x(chl)	y(chl)	QA1(chl)	Q1(chl)	Q4(chl)
		0.8830	0.6211	0.7011	0.2986	0.07934	0.1293

27g + 50mu + 20chl = 50bi + 10st + 75q + 61H2O

mode	g	mu	bi	st	chl	q	H2O	#
		0.3097		0.1194	0.1814	0.3398	0.04976	-#

more phase diagram calculations ?

To plot the line and point we copy the values from the tc-pseudotute-dr.txt file into the dr-project.txt file and set the reaction line to begin at the invariant point we just calculated (have a look at the finished project file or the first tutorial for help on this). Now run drawpd; because we have specified the file we want to draw in the prefs-file ("dr-prefs.txt") drawpd automatically plots our diagram. Open the resulting eps-file with any illustration-software of your choice.

The resulting diagram looks like the figure on the right:

Since we already know that both garnet and biotite are removed from the assemblage we can calculate the respective lines directly. Starting with the garnet-out line:

```
choose phases : g chl st bi <return>
```

```
fluid is just H2O
```

```
in excess: mu q H2O
```

```
.
```

```
. (not repeating the text here)
```

```
.
```

```
variance of required equilibrium (1?) : <return>
```

```
you may set zero modal proportions,
```

```
from: g mu bi st chl q H2O
```

```
which to set : g <return> (set g to 0)
```

```
calculate T at P (rather than P at T) ? <return>
```

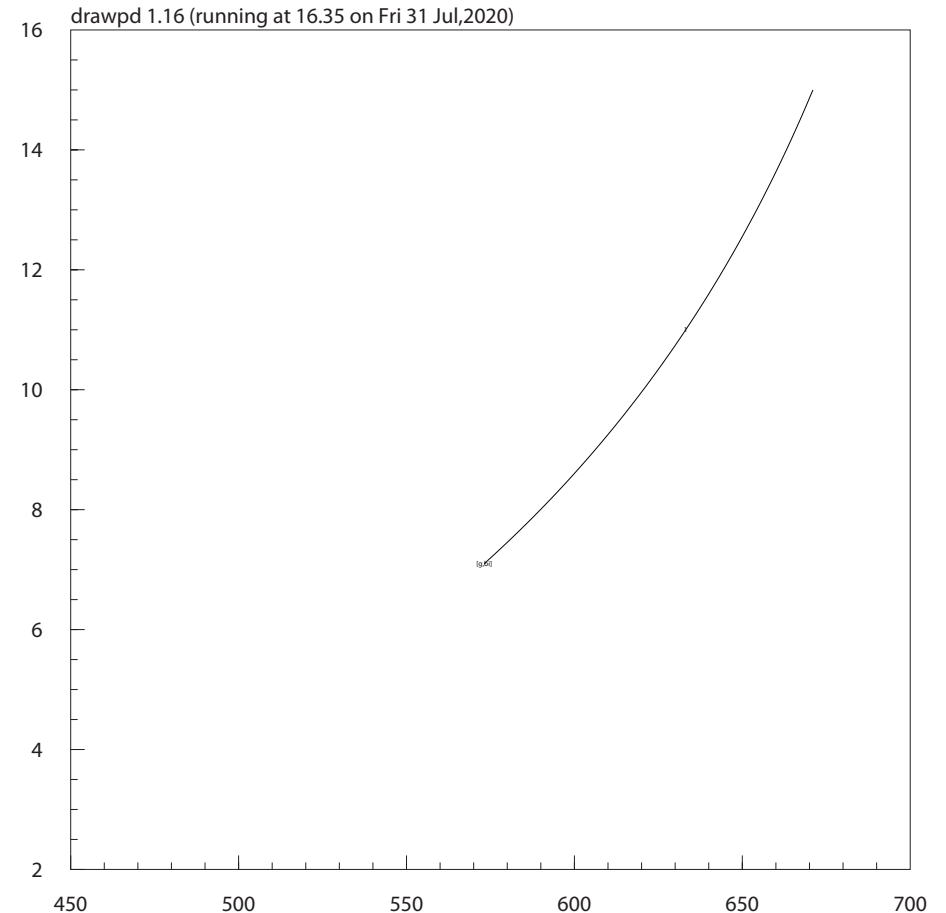
```
P calcs: between P(low) and P(high), with P increment : 7 12 0.1 <return>
```

```
...
```

```
composition (from bulk script)
```

H2O	SiO2	Al2O3	MgO	FeO	K2O
17.215	57.867	12.980	3.176	6.430	2.333

```
<=====>
```



phases: g bi st chl (mu, q, fluid)

88 (8 indicates that a phase is going to 0, in this case bi)

P (kbar)	T (°C)	x (g)	x (mu)	y (mu)	x (bi)	y (bi)	Q (bi)
7.200	575.12	0.9015	0.5584	0.9075	0.6975	0.2282	0.09601
		x (st)	x (chl)	y (chl)	QAl (chl)	Q1 (chl)	Q4 (chl)
		0.8766	0.6060	0.6974	0.3024	0.07896	0.1256

27g + 51mu + 21chl = 51bi + 10st + 76q + 62H2O

mode	g	mu	bi	st	chl	q	H2O	#
		0.2919	0.01858	0.1334	0.1578	0.3417	0.05658	-#

...

...

P (kbar)	T (°C)	x (g)	x (mu)	y (mu)	x (bi)	y (bi)	Q (bi)
8.000	589.88	0.8641	0.4842	0.8947	0.6008	0.2278	0.1194
		x (st)	x (chl)	y (chl)	QAl (chl)	Q1 (chl)	Q4 (chl)
		0.8233	0.4997	0.6697	0.3301	0.07321	0.09459

25g + 52mu + 22chl = 52bi + 10st + 78q + 69H2O

```

mode      g      mu      bi      st      chl      q      H2O      #
          0.1814   0.1344   0.2174   0.01429   0.3543   0.09824  -#

```

888888888888888888 (8 indicates that a phase is going to 0, in this case chl)

more phase diagram calculations ?

Same procedure for the biotite-out line (not bothering with *< return >*, you know what to do =):

which to set : bi

calculate T at P (rather than P at T) ?

specification of PT window:

P range over which T of reactions to be calculated

P window: P low,high : 7 12 0.1

...

phases: g bi st chl (mu, q, fluid)

88 (8 indicates that a phase is going to 0, in this case g)

```

-----
P (kbar)    T (°C)      x (g)      x (mu)      y (mu)      x (bi)      y (bi)      Q (bi)
    7.200    575.12    0.9015    0.5584    0.9075    0.6975    0.2282    0.09601
          x (st)      x (chl)      y (chl)    QAl (chl)    Q1 (chl)    Q4 (chl)
          0.8766    0.6060    0.6974    0.3024    0.07896    0.1256

```

27g + 51mu + 21chl = 51bi + 10st + 76q + 62H2O

mode	g	mu	bi	st	chl	q	H2O	#
	0.008991	0.3097		0.1198	0.1702	0.3379	0.05346	-#

...

...

P (kbar)	T (°C)	x (g)	x (mu)	y (mu)	x (bi)	y (bi)	Q (bi)
11.000	633.15	0.7243	0.3175	0.8483	0.3544	0.2058	0.1302
		x (st)	x (chl)	y (chl)	QAl (chl)	Q1 (chl)	Q4 (chl)
		0.6056	0.2713	0.6043	0.3954	0.04949	0.02248

19g + 57mu + 28chl = 57bi + 10st + 82q + 92H2O

mode	g	mu	bi	st	chl	q	H2O	#
	0.1461	0.3097		0.1252	0.0004722	0.3089	0.1096	-#

8888888888 (8 indicates that a phase is going to 0, in this case chl)

more phase diagram calculations ?

Now we plot the data and colour in the lines – look this up in the finished project file, in the first tutorial or in the [drawpd documentation](#). On the right is the result (note that I have zoomed-in the P - T interval):

You'll see that all reactions lie on top of each other. This means that the staurolite isograd is simultaneously the garnet-out towards high temperature and the biotite-out towards low temperature. This peculiarity is due to the isograd being an univariant reaction that separates divariant fields, implying that two phase change along the line, not just one. This makes things a little tricky to see, but it will become clearer as we proceed with the calculations.

From the calculations above we have learned that both the garnet-out and the biotite-out start from the *[garnet, biotite]*-invariant and that they terminate with chlorite going to 0. We can easily calculate the points with THERMOCALC, using the same recipe as above:

```
choose phases : g chl st bi
```

```
...
```

```
variance of required equilibrium (1?) :
```

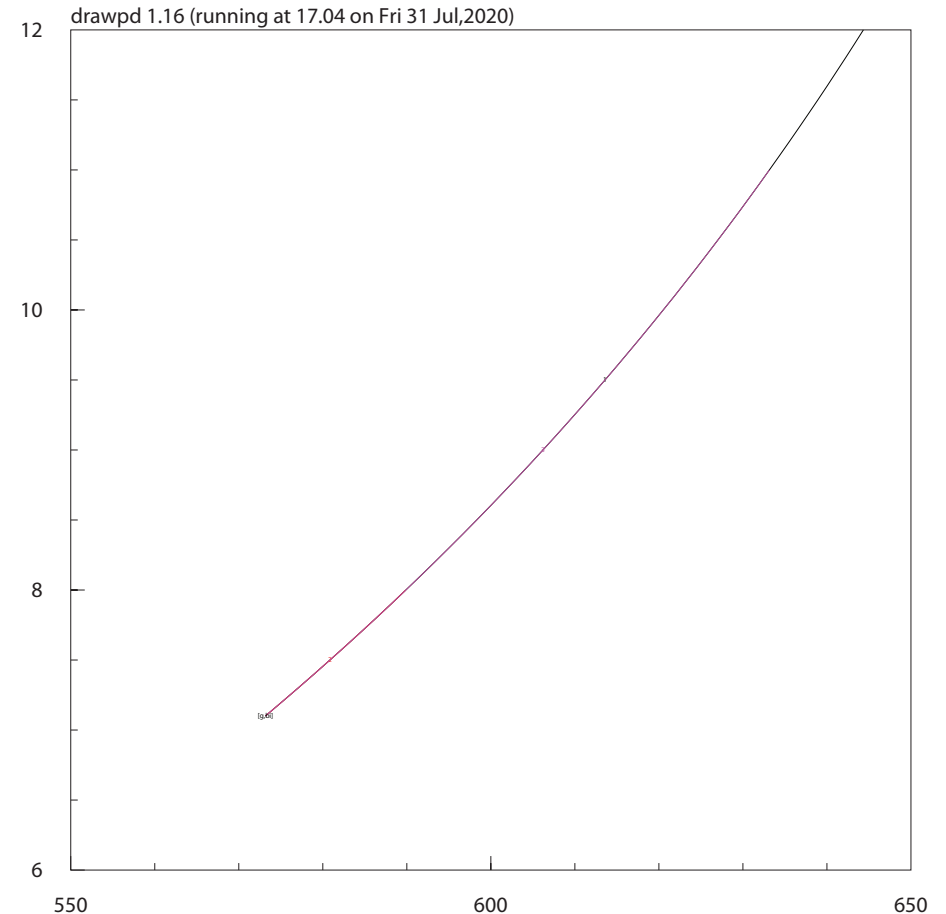
```
you may set zero modal proportions,
```

```
from: g mu bi st chl q H2O
```

```
which to set : g chl
```

```
...
```

```
phases: g bi st chl (mu, q, fluid)
```



P (kbar)	T (°C)	x (g)	x (mu)	y (mu)	x (bi)	y (bi)	Q (bi)
8.099	591.60	0.8595	0.4765	0.8932	0.5900	0.2276	0.1216
		x (st)	x (chl)	y (chl)	QAl (chl)	Q1 (chl)	Q4 (chl)
0.8166	0.4884	0.6666	0.3331	0.07236	0.09094		

25g + 53mu + 22chl = 53bi + 10st + 78q + 70H2O

mode	g	mu	bi	st	chl	q	H2O	#
		0.1701	0.1462	0.2256		0.3557	0.1024	-#

more phase diagram calculations ?

And:

phases: g bi st chl (mu, q, fluid)

P (kbar)	T (°C)	x (g)	x (mu)	y (mu)	x (bi)	y (bi)	Q (bi)
11.017	633.35	0.7235	0.3168	0.8481	0.3533	0.2056	0.1301
		x (st)	x (chl)	y (chl)	QAl (chl)	Q1 (chl)	Q4 (chl)
		0.6044	0.2704	0.6041	0.3956	0.04938	0.02225

19g + 57mu + 28chl = 57bi + 10st + 82q + 92H2O

```

mode      g      mu      bi      st      chl      q      H2O      #
          0.1465    0.3097          0.1252          0.3088    0.1098    -#

```

more phase diagram calculations ?

We have learned above that in this bulk, the staurolite isograd separates three divariant fields from each other, namely biotite–staurolite–chlorite, garnet–staurolite–chlorite and garnet–staurolite–biotite (+q +mu +H₂O). From the invariants we know that they each emanate phase-out lines, for example the field biotite–staurolite–chlorite is delimited by a biotite-out towards low temperature and a chlorite-out towards high temperature. This is how to calculate those, using the biotite-out as an example:

```
choose phases : bi st chl
```

```
...
```

```
variance of required equilibrium (2?) :
```

```
you may set zero modal proportions, from: mu bi st chl q H2O
```

```
which to set : bi
```

```
calculate T at P (rather than P at T) ?
```

```
specification of PT window:
```

```
P range over which T of reactions to be calculated
```

```
P window: P low,high : 2 8 0.1
```

```
...
```

```
phases: bi st chl (mu, q, fluid)
```

```

-----
P(kbar)      T(°C)      x(mu)      y(mu)      x(bi)      y(bi)      Q(bi)      x(st)
  2.000      519.14      0.5568      0.9622      0.7289      0.3366      0.08357      0.9061

```

x(chl)	y(chl)	QAl(chl)	Q1(chl)	Q4(chl)
0.6315	0.8278	0.1719	0.06505	0.1463



mode	mu	bi	st	chl	q	H2O	G #
	0.3097		0.08839	0.2110	0.3487	0.04215	-904.56203 #

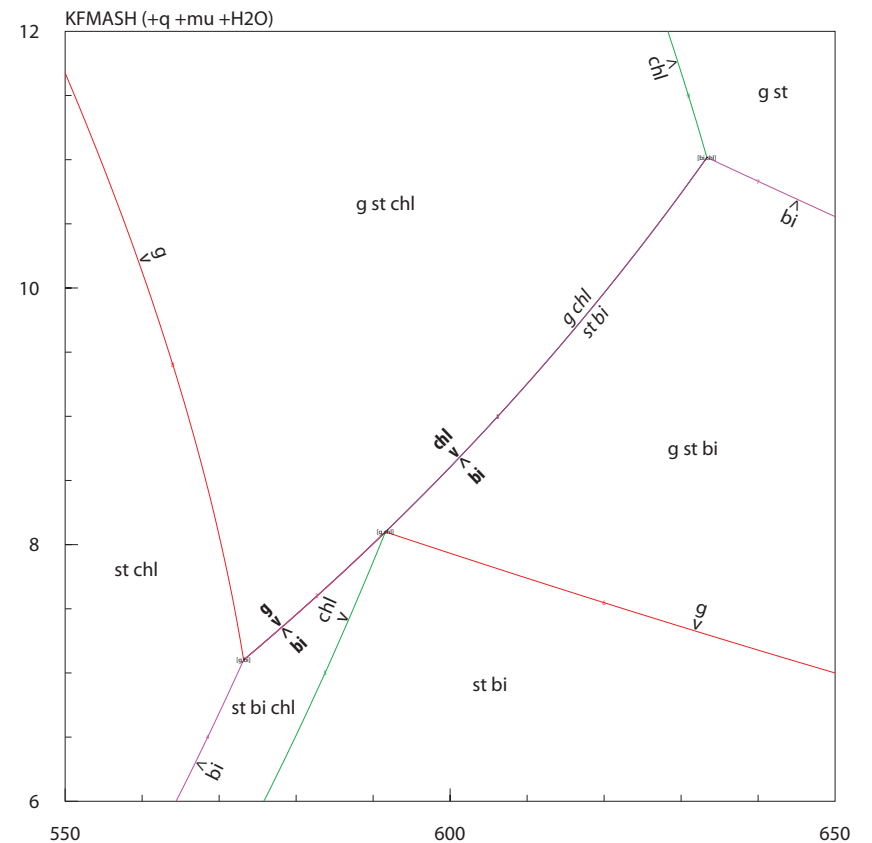
...

The chlorite-out is calculated the same way.

Similarly, the garnet–staurolite–chlorite and garnet–staurolite–biotite fields have a garnet-out towards lower temperature, as well as a chlorite-out and a biotite-out. This may sound confusing at first, but it comes directly from the invariants that we just calculated.

The result may look something like this the figure on the right. I coloured the lines for reference and manually added some field labels as well as reaction **1** in italics.

This figure neatly sums up what we have found out so far, in particular how univariant reactions serve as field boundaries. They can be seen as two overlapping phase-in and phase out boundaries (or as an infinitely narrow field) because the variance across the reaction remains constant (2), as well as the number of phases in neighbouring fields (3). This is exclusive to univariant reactions, since ‘normal’ field boundaries simply involve the appearance/disappearance of one phase (e.g.



the garnet-out in the figure to the right).

When calculating pseudosections for metapelites we can take advantage of the dominant KFMASH reactions that we have calculated in the first tutorial (or from publications). This is the method follows the steps as we have done until now, i.e. calculate a univariant reaction (such as the staurolite isograd) and look where it is 'seen' by the chosen bulk composition. However, this only works for small systems and metapelites that are based on a strong backbone system such as KFMASH.

An other useful method is to use THERMOCALC to find the most stable assemblage at a given P - T with the *dogmin* facility. Here is an example of how that works. We are looking for the most stable assemblage at 10 kbar & 550 °C:

First, you need to activate the keyword in the scriptfile by removing the %:

```
dogmin 0
```

Then, run THERMOCALC:

```
choose phases : g chl ctd st bi ky (phases that might be stable)
```

```
...
```

```
max variance of equilibria to be looked at : 5 (variance that is explored)
```

```
specification of PT calcs:
```

```
P at which equilibria to be calculated
```

```
P calcs: between P(low) and P(high), with P increment : 10 (pressure of interest)
```

```
T at which equilibria to be calculated
```

```
T calcs: between T(low) and T(high), with T increment : 550 (temperature of interest)
```

```
specification of bulk composition
```

```
composition (from bulk script)
```

H2O	SiO2	Al2O3	MgO	FeO	K2O
17.215	57.867	12.980	3.176	6.430	2.333

#####

Gibbs energy minimisation gives the trivariant assemblage mu chl ctd q H2O
with, in excess, mu q H2O, also trying assemblages involving g bi st ky

P (kbar)	T (°C)	x(mu)	y(mu)	x(chl)	y(chl)	QAl(chl)	Q1(ch#
10.0000	550.000	0.4545	0.8939	0.4757	0.6654	0.3345	0.075#
		Q4(chl)	x(ctd)				
		0.09143	0.8204				

mode	mu	chl	ctd	q	H2O
	0.3097	0.0898	0.2230	0.3399	0.0376

From this we learn that at 10 kbar & 550°C, the most stable assemblage is chloritoid–chlorite (+q +mu +H₂O). Technically you could repeat this procedure at different *P–T* points and calculate the full pseudosection. This is actually how both Theriak and Perple_X calculate pseudosections, by so called *ΔG–minimization*. For more information on this see the [documentation](#) and the files that can be downloaded there with tips on how to obtain the correct answer with dogmin.

Alright, from this and the figure above we now know that the assemblage staurolite–chlorite becomes chloritoid–chlorite (both +q +mu +H₂O) somewhere above 550°C. The garnet-out of the garnet–staurolite–chlorite field therefore runs into the chloritoid-stability field towards low temperature. We can calculate this point in THERMOCALC! First we need to deactivate the *dogmin* keyword in the scriptfile, though:

```
%dogmin 0
```

In THERMOCALC:

choose phases : g st chl ctd

...

variance of required equilibrium (1?) : (variance of 1 rings a bell!)

you may set zero modal proportions, from: g mu st chl ctd q H2O

which to set : g ctd

phases: g st chl ctd (mu, q, fluid)

P (kbar)	T (°C)	x (g)	x (mu)	y (mu)	x (st)	x (chl)	y (chl)
8.974	566.11	0.9086	0.5653	0.8966	0.8832	0.6188	0.6819
		QA1 (chl)	Q1 (chl)	Q4 (chl)	x (ctd)		
		0.3179	0.08335	0.1289	0.8746		

536ctd + 144q = 101g + 47st + 10chl + 402H2O

mode	g	mu	st	chl	ctd	q	H2O	#
		0.3097	0.1245	0.1765		0.3383	0.05102	-#

The assemblage involving garnet–staurolite–chlorite–chloritoid (+q +mu +H₂O) is that of a univariant reaction that we calculated in the first tutorial, it defines the *terminal breakdown* of chloritoid:



Because this reaction does not involve muscovite nor biotite, it exists in the K₂O-absent subsystem of FMASH and is a so-called *degenerate* reaction.

We have met this type of reactions in the first tutorial – if it sounds unknown you can look it up there or in any petrology textbook.

You could calculate this reaction exactly as we have done with the staurolite isograd, or calculate the lines emanating from the $[g, ctd]$ invariant point from above. For example, the garnet-out:

choose phases : **g st chl ctd**

variance of required equilibrium (1?) :

you may set zero modal proportions, from: g mu st chl ctd q H2O

which to set : **g**

calculate T at P (rather than P at T) ?

specification of PT window:

P range over which T of reactions to be calculated

P window: P low,high : **8 12 0.1**

...

phases: g st chl ctd (mu, q, fluid)

8888888888 (these are telling us that the amount of a phase runs to 0 towards low P, here it is chloritoid)

P(kbar)	T(°C)	x(g)	x(mu)	y(mu)	x(st)	x(chl)	y(chl)
9.000	566.24	0.9081	0.5640	0.8962	0.8825	0.6171	0.6813
QA1(chl)	Q1(chl)	Q4(chl)	x(ctd)				
0.3185	0.08337	0.1285	0.8739				

534ctd + 143q = 100g + 47st + 10chl + 401H2O

mode	g	mu	st	chl	ctd	q	H2O	#
		0.3097	0.1227	0.1750	0.003487	0.3383	0.05083	-#

...

The 8 output tells us that from this point a chloritoid-out runs towards low pressure, but without garnet:

last time was: g st chl ctd + mu q H2O

choose phases : -g (removing garnet from the previous assemblage)

...

variance of required equilibrium (2?) :

you may set zero modal proportions, from: mu st chl ctd q H2O

which to set : ctd

calculate T at P (rather than P at T) ?

specification of bulk composition

composition (from bulk script)

H2O	SiO2	Al2O3	MgO	FeO	K2O
17.215	57.867	12.980	3.176	6.430	2.333

<=====>

phases: st chl ctd (mu, q, fluid)

P (kbar)	T (°C)	x(mu)	y(mu)	x(st)	x(chl)	y(chl)	QAl(chl)
2.000	467.20	0.5382	0.9810	0.9228	0.6377	0.8986	0.1012

Q1(chl)	Q4(chl)	x(ctd)
0.05898	0.1607	0.9210

417ctd + 108q = 74g + 37st + 10chl + 304H2O

mode	mu	st	chl	ctd	q	H2O	G #
	0.3097	0.07072	0.2280		0.3538	0.03781	-899.15976 #

...

The garnet-out calculated above terminates with a string of 8 towards higher pressure:

...

P (kbar)	T (°C)	x (g)	x (mu)	y (mu)	x (st)	x (chl)	y (chl)
11.3000	576.568	0.8652	0.4663	0.8681	0.8164	0.4802	0.6350
		QA1(chl)	Q1(chl)	Q4(chl)	x(ctd)		
		0.3648	0.08069	0.08828	0.8044		

mode	g	mu	st	chl	ctd	q	H2O	#
		0.3097	0.003410	0.08088	0.2291	0.3380	0.03892	-#

8888888 (we see that the staurolite-mode tends towards 0)

more phase diagram calculations ?

This tells us that the reaction terminates in a point where staurolite becomes 0. We calculate it easily:

choose phases : g st chl ctd

...

variance of required equilibrium (1?) :

you may set zero modal proportions, from: g mu st chl ctd q H2O

which to set : g st

...

phases: g st chl ctd (mu, q, fluid)

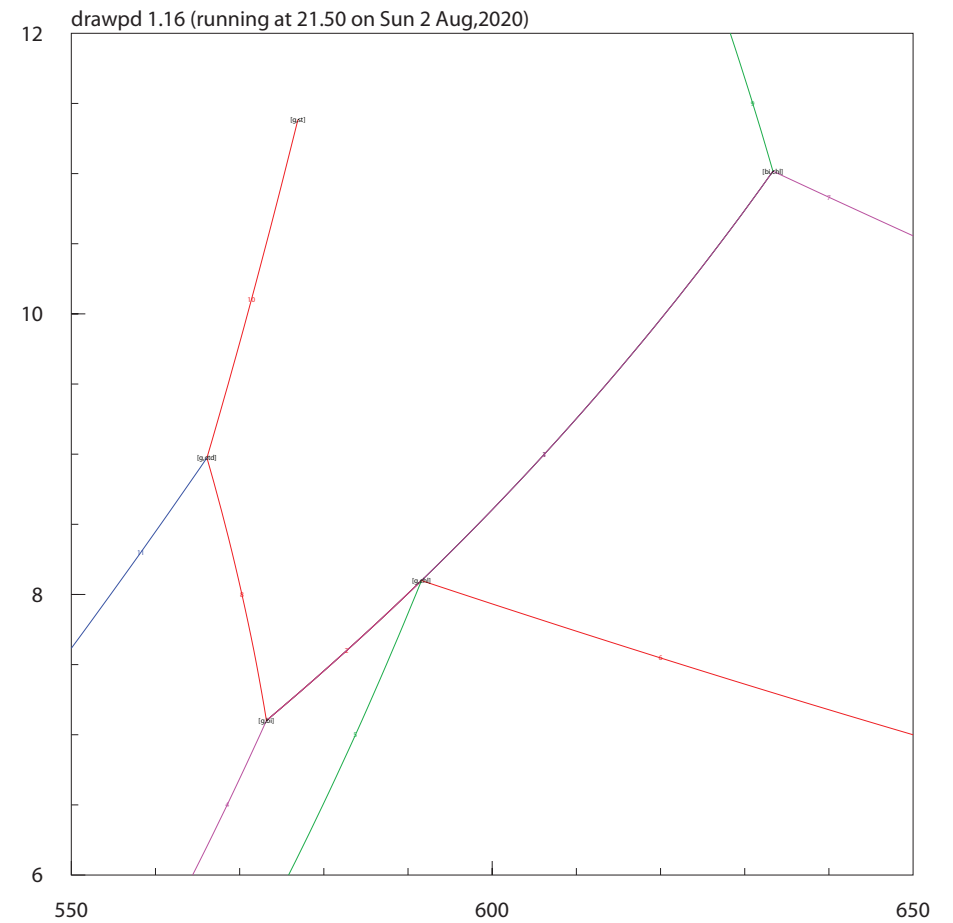
P (kbar)	T (°C)	x (g)	x (mu)	y (mu)	x (st)	x (chl)	y (chl)
11.385	576.92	0.8636	0.4631	0.8670	0.8137	0.4756	0.6335
		QAl (chl)	Ql (chl)	Q4 (chl)	x (ctd)		
		0.3663	0.08046	0.08679	0.8017		

414ctd + 107q = 74g + 36st + 10chl + 301H2O

mode	g	mu	st	chl	ctd	q	H2O	#
		0.3097		0.07823	0.2355	0.3380	0.03858	-#

more phase diagram calculations ?

If we assemble the lines and points that we have just calculated, we get something like this:



There are some crucial spots, one of them being the stability field for the aluminosilicates. The triple point and the lines can be calculated as we have done until now. First, the point. You simply need to specify an assemblage that contains all three aluminosilicates plus two other phases to make an invariant assemblage:

• • •

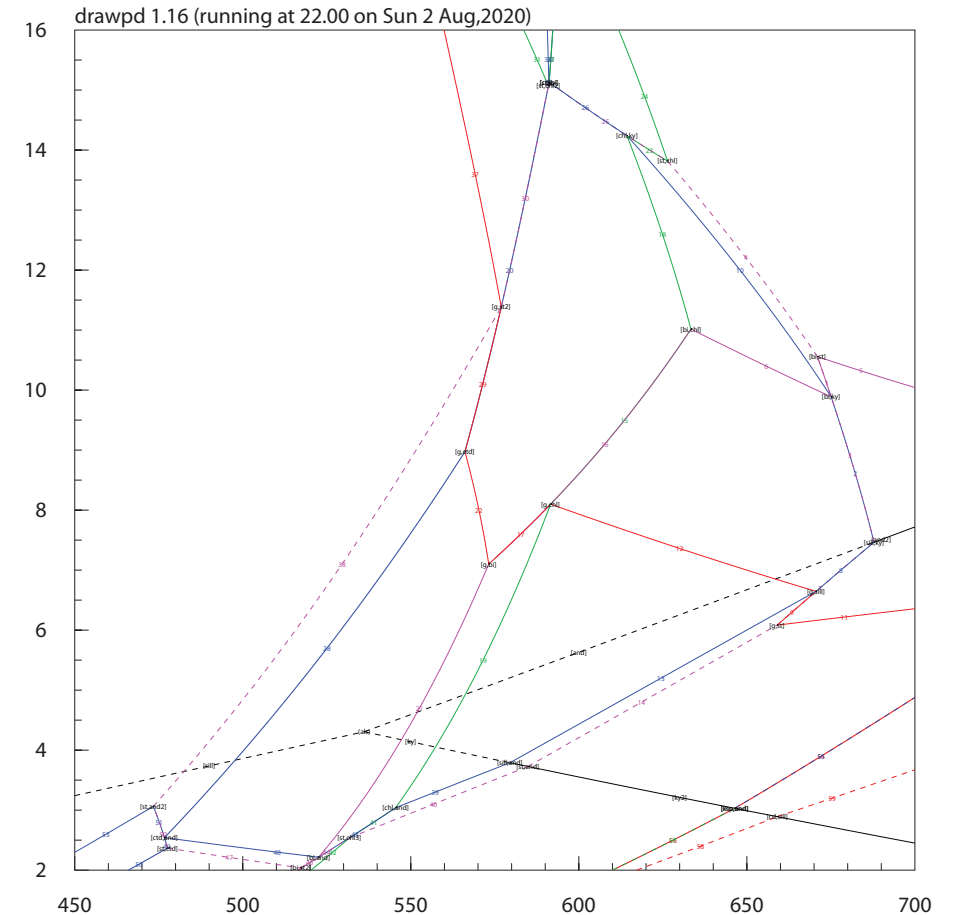
...

using overall PT window for the PT window

composition (from bulk script)

H2O	SiO2	Al2O3	MgO	FeO	K2O
17.215	57.867	12.980	3.176	6.430	2.333

<=====>



P (kbar)	T (°C)	x (g)	x (mu)	y (mu)	x (cd)	h (cd)
4.307	536.19	0.8267	0.3652	0.9302	0.2268	0.7775

414ctd + 107q = 74g + 36st + 10chl + 301H2O

more phase diagram calculations ?

I added garnet and cordierite to the assemblage, but this is not important because the point is defined by the phase relations of the aluminosilicates. They are another example of a degenerate equilibrium, implying that the phase transitions will occur in any compositional system, provided it contains Al₂O₃ and SiO₂. Then, for example, the andalusite–kyanite transition:

last time was: g cd sill and ky + mu q H2O (same as before)

choose phases : -sill (remove sill)

variance of required equilibrium (1?) :

you may set zero modal proportions, from: g mu cd and ky q H2O

which to set : ky

calculate T at P (rather than P at T) ? no

specification of PT window:

T range over which P of reactions to be calculated

T window: T low,high : 450 550 5

phases: g cd and ky (mu, q, fluid)

P (kbar)	T (°C)	x (g)	x (mu)	y (mu)	x (cd)	h (cd)
3.242	450.00	0.8691	0.3353	0.9446	0.2100	0.7597

ky = and

mode	g	mu	cd	and	ky	q	H2O	#
	0.1400	0.3097	0.1336	0.03347		0.2740	0.1093	-#

...

The other two lines are calculated similarly.

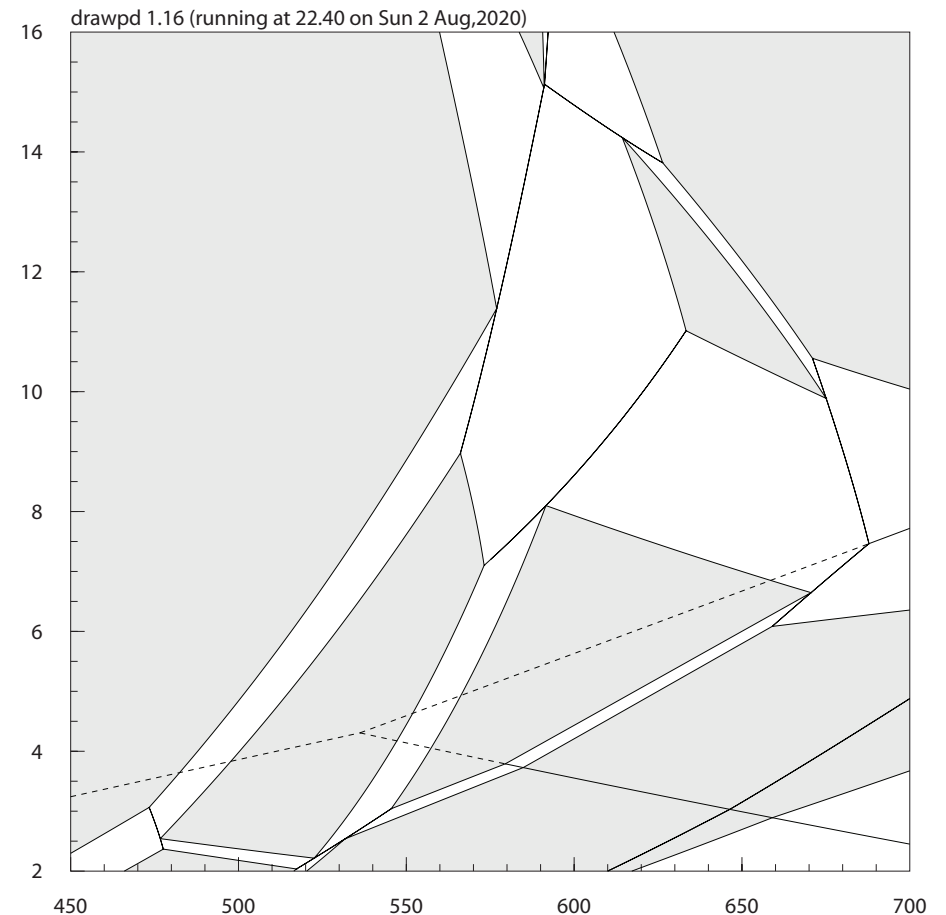
Once the diagram is calculated we can use drawpd to fill the assemblage fields. For this, scroll down to the bottom of your -dr-file and specify the shade and the lines that make up a field, for example:

```
0.65 u53 u38 u37
```

Here 0.65 defines the shade (choose between 0–1, from darkest to brightest) and u53 u38 u37 are three lines that define a triangle. Traditionally, the higher the variance of a field, the darker the shading. You can choose a RGB colour by changing the code

```
darkcolour 192 192 192
```

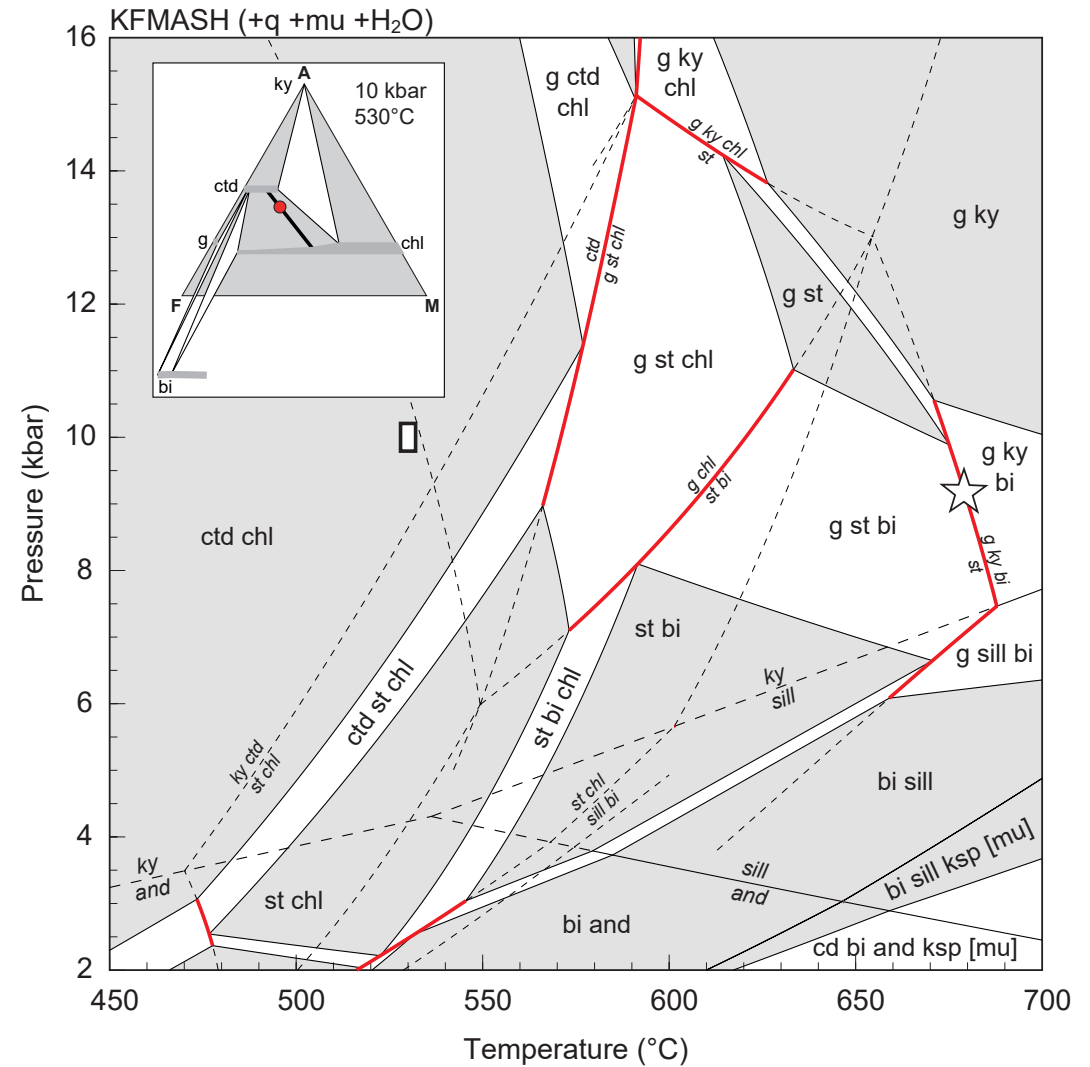
For diagram to the right I coloured the fields – which all are divariant (white) and trivariant (grey) – and removed the colour from the lines in the dr-file. All we need to do now is adding labels.

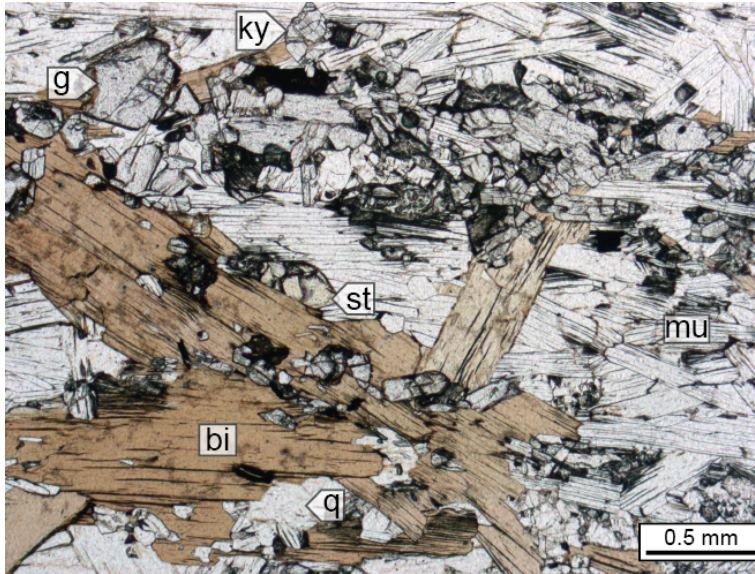


The relationship of P - T projection, compatibility diagram and pseudosection

The final figure illustrates that a pseudosection contains part of the information of the P - T projection, but distilled through the chosen bulk composition. The red lines are univariant reactions that our bulk sees. This makes pseudosections tailored tools for understanding the evolution of a specific rock, whereas the P - T projection shows the phase relations that are stable in a given system (here KFMASH) as a function of P - T .

The compatibility diagram is calculated at 10 kbar & 550 °C and shows the phase relations stable at this P - T as well as the assemblage expressed by the specified bulk composition (red dot; see tutorial II for more information on this). The AFM plot tells us that at 10 kbar & 550 °C, this bulk would produce the assemblage chlorite–chloritoid (+mu +q +H₂O) – as reflected in the pseudosection.





This is a thin section of sample A33, for which we have calculated the pseudosection in this tutorial. It contains the main assemblage of garnet–biotite–staurolite–kyanite–muscovite–quartz if we ignore minor plagioclase and ilmenite. Assuming H_2O saturation during equilibration, we see that this assemblage exactly corresponds to the terminal breakdown-reaction of staurolite in the KFMASH system:



The pseudosection above tells us that in this bulk composition, the assemblage is stable over a very narrow P – T interval, about 8–10 kbar & 670–690 °C (approximated by the white star above). How about that, we have just applied pseudosection thermobarometry to estimate the equilibration conditions of an actual rock!

This P – T estimate is essentially identical to the one determined using the much more complex MnO – Na_2O – CaO – K_2O – FeO – MgO – Al_2O_3 – SiO_2 – H_2O – TiO_2 – O_2 (MnNCKFMASHTO) model system. This reveals another key peculiarity of the metapelite system: the underlying KFMASH phase relations are dominant in all systems, and adding more components does not necessarily make a difference. However, the reaction corresponding to the assemblage would become a narrow multivariant field. This proves that more complicated doesn't automatically mean better. KFMASH's not dead!

Tips and tricks for smooth calculations

Starting guesses

When calculating diagrams with THERMOCALC, sometimes it can happen that you are trying to calculate points or lines that should exist, but the program refuses to calculate them and frustrates you with an output of 7777. Watch out for these!

Here's an example using the bulk in this tutorial: I'm looking for the $[bi, st]$ invariant point at low pressure:

```
choose phases : bi st chl and
```

```
variance of required equilibrium (1?) :
```

```
you may set zero modal proportions, from: mu bi st chl and q H2O
```

```
which to set : bi st
```

```
specification of PT window:
```

```
PT window within which invariant points expected to lie
```

```
T low,high, P low,high :
```

```
composition (from setbulk script)
```

H2O	SiO2	Al2O3	MgO	FeO	K2O
17.215	57.867	12.980	3.176	6.430	2.333

```
<=====>
```

```
phases: bi st chl and (mu, q, fluid)
```

```
7<== nothing in range ==>
```

```
more phase diagram calculations ?
```

This means that THERMOCALC has tried to calculate the point, but wasn't able to find it. This is related to something called *starting guesses*. They are the numbers at the bottom of the scriptfile:

```
% -----  
% at P = 6.5, T = 561, for: g mu bi st chl q H2O  
% -----  
ptguess 6.500 560.78  
% -----  
xyzguess x(g)          0.934933  
% -----  
xyzguess x(mu)         0.650219  
xyzguess y(mu)         0.919549  
% -----  
xyzguess x(bi)         0.795109  
xyzguess y(bi)         0.225772  
xyzguess Q(bi)         0.0667504  
% -----  
xyzguess x(st)         0.921385  
% -----  
xyzguess x(chl)        0.723911  
xyzguess y(chl)        0.725999  
xyzguess QAl(chl)      0.273769  range -1.000 1.000  
xyzguess Q1(chl)       0.0776481 range -1.000 1.000  
xyzguess Q4(chl)       0.145937  range -1.000 1.000  
% -----
```

They tell THERMOCALC in what compositional space to start ‘looking’ when performing calculations. If the set numbers are too far off the equilibrium you are looking for, the calculation might fail and you get the 7 flag. To solve this problem you need to specify starting guess that lie closer to the wanted equilibrium. For this, open the tc-log.txt file and look for a successful calculation near the P – T conditions where the calculation previously failed. For example:

```
% -----
% at P = 3.0, T = 534, for: mu bi st chl q H2O  with bi = 0
% -----
ptguess 3.0 534
% -----
xyzguess x(mu)          0.560851
xyzguess y(mu)          0.953860  range  0.000 2.000
% -----
xyzguess x(bi)          0.724585
xyzguess y(bi)          0.315239
xyzguess Q(bi)          0.0852917
% -----
xyzguess x(st)          0.900564
% -----
xyzguess x(chl)         0.629655
xyzguess y(chl)         0.804903
xyzguess QAl(chl)       0.194819  range -1.000 1.000
xyzguess Q1(chl)        0.0671977 range -1.000 1.000
xyzguess Q4(chl)        0.142383  range -1.000 1.000
% -----
```

Copy and paste the new numbers above the previous starting guesses, and try to calculate the point again:

choose phases : `bi st chl and`

variance of required equilibrium (1?) :

you may set zero modal proportions, from: `mu bi st chl and q H2O`

which to set : `bi st`

...

phases: `bi st chl and (mu, q, fluid)`

```
-----
P (kbar)      T (°C)      x(mu)      y(mu)      x(bi)      y(bi)      Q(bi)      x(st)
  2.0361      517.279      0.5875      0.9625      0.7603      0.3293      0.07434     0.9180
                x(chl)      y(chl)      QAl(chl)      Q1(chl)      Q4(chl)
                0.6709      0.8294      0.1703      0.06971      0.1540

mode          mu          bi          st          chl          and          q          H2O      #
              0.3097                0.2472      0.06457      0.3419      0.03660     -#
```

more phase diagram calculations ?

Done and done!

c8 keyword

Above we often have encountered calculations that abruptly terminate with a string of 888, flagging that a phase mode is running towards 0. Sometimes it can be confusing to see what phase exactly is running out. To make it visible you can activate the `c8` keyword in the scriptfile:

c8 yes

Using the garnet-out of the garnet–biotite–staurolite–chlorite assemblage from above as an example:

choose phases : g bi st chl

variance of required equilibrium (1?) :

you may set zero modal proportions, from: g mu bi st chl q H2O

which to set : g

calculate T at P (rather than P at T) ?

specification of PT window:

P range over which T of reactions to be calculated

P window: P low,high : 8 9

T window within which reactions expected to lie

T window: T low,high :

use the P interval in the datafile script ?

P interval = 0.1 (from script)

composition (from setbulk script)

H2O	SiO2	Al2O3	MgO	FeO	K2O
17.215	57.867	12.980	3.176	6.430	2.333

<=====>

phases: g bi st chl (mu, q, fluid)

...

P (kbar)	T (°C)	x (g)	x (mu)	y (mu)	x (bi)	y (bi)	Q (bi)
8.0000	589.885	0.8641	0.4842	0.8947	0.6008	0.2278	0.1194
		x (st)	x (chl)	y (chl)	QAl (chl)	Q1 (chl)	Q4 (chl)
		0.8233	0.4997	0.6697	0.3301	0.07321	0.09459

27g + 51mu + 21chl = 51bi + 10st + 76q + 64H2O

mode	g	mu	bi	st	chl	q	H2O	#
		0.1814	0.1344	0.2174	0.01429	0.3543	0.09824	-#

P (kbar)	T (°C)	x (g)	x (mu)	y (mu)	x (bi)	y (bi)	Q (bi)
8.1000	591.617	0.8595	0.4764	0.8932	0.5899	0.2276	0.1216
		x (st)	x (chl)	y (chl)	QAl (chl)	Q1 (chl)	Q4 (chl)
		0.8165	0.4883	0.6666	0.3332	0.07235	0.09090

27g + 51mu + 21chl = 51bi + 10st + 76q + 64H2O

mode	g	mu	bi	st	chl	q	H2O	#
#		0.1700	0.1464	0.2257-0.0001546		0.3557	0.1024	-#

(chlorite-mode becomes negative, marking it as the phase that runs out)