

Introduction to phase diagram calculations in KFMASH – tutorial II

by Simon Schorn (December 21, 2020)

This is the second of three tutorials, designed to give you a brief introduction to phase diagram calculations using THERMOCALC. Here we look into AFM compatibility diagrams. This tutorial follows up on the previous lesson dealing with P – T projections 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 v3.50 (version from dec 2020; see THERMOCALC [download guide](#) and [downloads](#) on the webpage). The download-folder contains a simple Excel-spreadsheet for triangular plots and a compilation of finished AFM diagrams is added at the end of this file.

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

tc350	THERMOCALC executable
tc-prefs	THERMOCALC preferences file (prefsfile)
tc-AFM	script file (scriptfile)
tc-ds62	thermodynamic dataset
tc-mp50KFMASH	activity–composition file (axfile)

The file tc-prefs contains the following:

```
dataset 62
```

```
calcmode 1
scriptfile AFM
```

for THERMOCALC to automatically use this script file, and specifying you are doing phase diagram calculations.

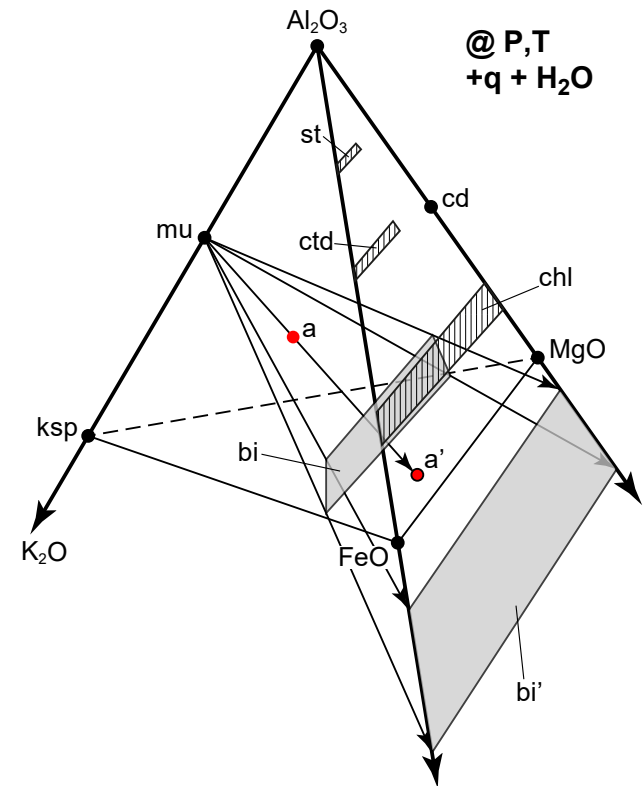
You are good to go!

Introduction to AFM compatibility diagrams

The plotting of compatibility diagrams is a general method, but we will use the example of *AFM* (Al_2O_3 – FeO – MgO) *diagrams* which are very useful for understanding metapelites. This method was introduced by Thompson (1957) in a seminal paper (The graphical analysis of mineral assemblages in pelitic schists. *AmMin*, 42, 11–12) and is commonly used since then. Generally speaking, compatibility diagrams are triangular graphs used to represent mineral assemblages in (metamorphic) rocks at specified P and T . In addition, they show the stable assemblage a given bulk rock composition would produce at these conditions.

Because rocks and minerals commonly consist of a number of chemical components (6 in the simplified KFMASH system), not all of them can be graphically represented on a piece of paper. In fact, if we were to draw a compositional diagram, best we could do is a 4-component compatibility tetrahedron, like the one shown on the right.

Here we take advantage of the abundance of quartz (q) and H_2O in subsolidus metapelites and assume that these two phases are always present, as we have done for the P – T projection in the previous tutorial. In this case the vertices are given by the components K_2O – FeO – MgO – Al_2O_3 (KAFM), with SiO_2 and H_2O taken care of by



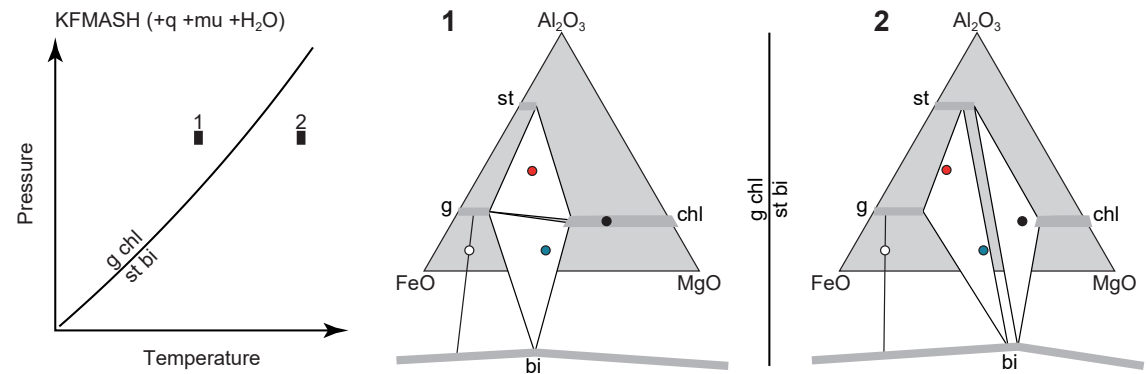
quartz and H₂O in excess.

Phases that nominally contain no K₂O fall directly onto the Al₂O₃–FeO–MgO-plane, for example chloritoid (ctd), staurolite (st) and chlorite (chl). Because these phases may contain variable amounts of these components, they occupy an area in compositional space. Phases having a fixed composition are shown as a dot, for example K-feldspar (ksp). Minerals, and bulk compositions however may contain all four of KAFM plus SiO₂ and H₂O, and therefore fall within the volume of the tetrahedron. Biotite and the composition *a* are examples.

To make our life easier, we reduce the dimensions of the tetrahedron to a triangle by taking advantage of the ubiquitous presence of muscovite in common metapelites. Phases falling within the KAFM volume are ‘projected’¹ from muscovite onto the AFM plane, implying that muscovite too is always present. As shown by the arrows, this causes *a*’ and *bi*’ to fall at different AFM-locations, with *bi*’ even having negative Al₂O₃ coordinates (assuming that the FeO–MgO join is the origin).

The figure on the right starts with a simplified representation of the staurolite isograd we met in the previous tutorial. Up temperature, it involves the reaction of garnet + chlorite → staurolite + biotite (plus muscovite, quartz and H₂O in excess).

The staurolite isograd is an univariant reaction, because it involves 7 phases in the 6-component system of KFMASH. The fields separated by it therefore are divariant, and as such must involve 6 phases. This relationship is given by the phase rule, and if this sounds completely unfamiliar you can look it up in any petrology textbook or the previous tutorial.



On the low-temperature side of the isograd (*PT*-point 1), garnet and chlorite may be joined by one of the phases on the other side of the reaction, so either by staurolite OR biotite – but staurolite AND biotite can never be stable on the left-hand side of the reaction. The *P–T*

¹Note that this is a geometric operation and not to be confused with true projections such as *P–T* projections.

projection however does not tell us which one of the possible assemblages will be seen by the rock. This is what compatibility diagrams are for.

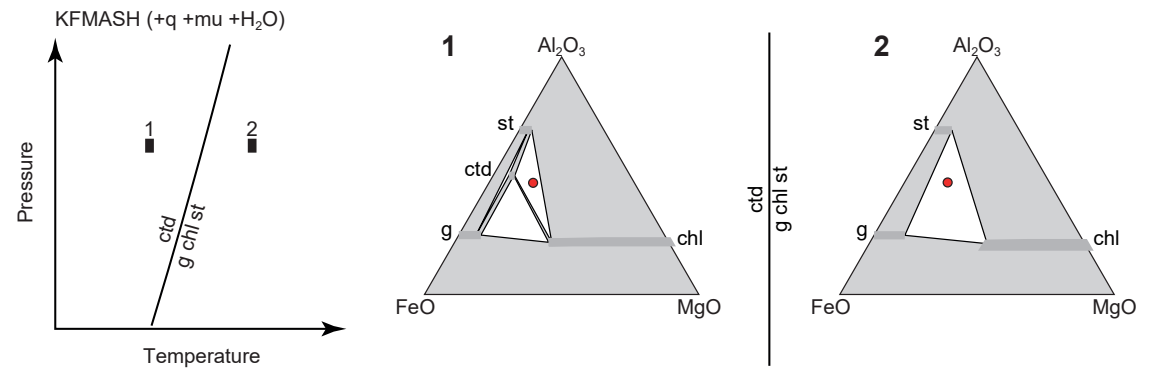
The respective AFM diagram drawn at fixed P - T (1) puts this into context: garnet and chlorite form one triangle with staurolite and another with biotite. The composition of phases is function of P - T and defined by the vertices of the triangles.

The coloured dots represent different bulk compositions, each with it's own AFM-ratio (such as a and a' above): the red bulk composition would produce the assemblage of garnet–chlorite–staurolite ($+mu +q +H_2O$), whereas the less aluminous blue bulk falls inside the other triangle, making garnet–chlorite–biotite ($+mu +q +H_2O$). The white bulk falls into the field where garnet and biotite are coexisting, forming the trivariant assemblage of garnet–biotite ($+mu +q +H_2O$), whereas the black bulk plots into the area occupied by chlorite. Therefore, this bulk would 'make' the quadrivariant assemblage of chlorite ($+mu +q +H_2O$). This highlights that different rock compositions can form quite different assemblages at the same P - T conditions. The key here is to understand that it is not a specific mineral that is characteristic for certain P - T condition, but always the assemblage of minerals.

Now, we cross the staurolite isograd by isobaric heating to PT -point 2. On the high-temperature side of the reaction staurolite and biotite may coexist with garnet OR chlorite, but garnet and chlorite are not stable together. This is shown by the new triangles: one connects staurolite–biotite–garnet and the other staurolite–biotite–chlorite (both $+mu +q +H_2O$). We see that now both the red and blue bulk fall within the first triangle, implying that both bulks would produce the same assemblage, but with a different mineral ratio. The white bulk on the other hand would not change its assemblage, still consisting of garnet–biotite ($+mu +q +H_2O$).

However, because we are now looking at different $(P)T$, the mineral composition would be different as shown by the slightly different orientation of the line connecting the two. The latter is a so-called *tieline*. The former chlorite-assemblage of the black bulk now lies in the second triangle, meaning that it contains the divariant assemblage of staurolite–biotite–chlorite ($+mu +q +H_2O$).

This was an example of a *cross-tieline reaction*, the other case is the *terminal breakdown reaction*, for example the chloritoid-breakdown as shown on the right. On the low- T side (PT -point 1) chloritoid can form divariant assemblages (triangles on the AFM plot) with two out of garnet, chlorite or staurolite. The red bulk would form chloritoid–chlorite–staurolite (+mu +q +H₂O) in this case.

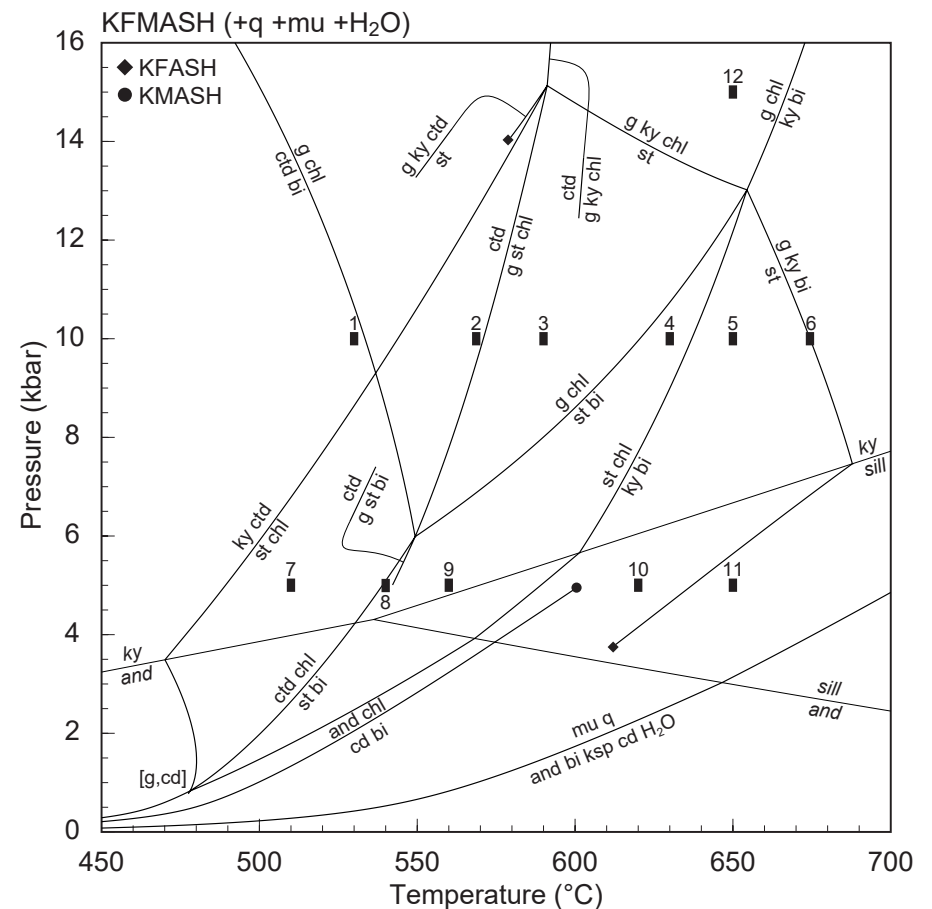


However, on the high- T side of the reaction (point 2) there already are three minerals to form a divariant assemblage. Chloritoid completely (terminally) breaks down and gives way to garnet–chlorite–staurolite (+mu +q +H₂O) in case of the red bulk. The terminal breakdown of staurolite at upper-amphibolite facies conditions shows the same behaviour.

AFM compatibility diagrams in THERMOCALC

Calculating compatibility diagrams in THERMOCALC is pretty straightforward. However, the data cannot be plotted using drawpd. You can draw your diagrams using any kind of triangular plots – in Excel using the attached AFMplot.xls, online or even on a simple sheet of paper. I plot them in Excel and then redraw them using an illustration software.

Here is the P – T projection that we made in the previous tutorial, with



the labels showing the P - T conditions where AFM diagrams are calculated. A compilation of plots can be found at the end of this tutorial.

I added a bulk composition for an amphibolite-facies aluminous meta- pelite from the Eastern Alps to the scriptfile. This is to show that the calculated assemblages are actually real and do occur in nature!

Now, let's fire up THERMOCALC! Note that user-input is highlighted in red and comments in blue.

When executing the program, you will see:

```
THERMOCALC 3.50 running at 17.59 on Wed 29 Jul,2020
using tc-ds62.txt produced at 20.08 on Mon 6 Feb,2012
with axfile tc-mp50KFMASH.txt and scriptfile tc-AFM.txt
```

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

```
with someof: g mu bi cd st chl ctd ky q H2O (from script)
inexcess: mu q H2O - auto included (from script)
choose phases :
```

This is where you will need to specify the phases that are part of the assemblage 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 in the scriptfile.

At point 1 (10 kbar & 530 °C) we are on the low-temperature side of the reactions chloritoid + biotite → garnet + chlorite and kyanite + chloritoid → staurolite + chlorite. We start with the divariant assemblage:

```
which phases : ctd bi g <return>
```

variance of required equilibrium (2?) : `<return>` (THERMOCALC correctly predicts a variance of 2)

specification of PT calcs:

P at which equilibria to be calculated

P calcs: between P(low) and P(high), with P increment : 10

T at which equilibria to be calculated

T calcs: between T(low) and T(high), with T increment : 530

Given that this *PT* information will be used for other calculations relating to this AFM diagram, it is convenient to include it in the scriptfile: “calcp 10”, and “calcT 530”, on separate lines after the “diagramPT” script.

projection plane has 3 apices, leaving H2O SiO2 Al2O3 MgO FeO K2O

to be represented by mu q H2O and the projection plane (mu, q, H2O set in excess previously)

projection plane (from script) (here the AFM projection plane is defined)

	H2O	SiO2	Al2O3	MgO	FeO	K2O
a	0	0	1.000	0	0	0
f	0	0	0	0	1.000	0
m	0	0	0	1.000	0	0

specification of bulk composition

composition (from script)

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

(KFMASH bulk for sample A33 in Schorn (2018), JMG)

<=====>

phases: g bi ctd (mu, q, fluid)

```

-----
P (kbar)      T (C)      x (g)      x (mu)      y (mu)      x (bi)      y (bi)      Q (bi)      x (ctd)
10.0000      530.000      0.9816      0.8518      0.8539      0.9376      0.08937      0.02366      0.9769

proj          a          f          m          q          H2O          mu          phase
g             0.2500      0.7362      0.0138      0.7500                                -0.2500
bi            -0.3823      1.3023      0.0800      -0.1177                                0.5000      -0.5000
ctd           0.5000      0.4885      0.0115      0.5000      0.5000                                -0.5000
(a, f, m are the coordinates we need!)

```

You can find the AFM coordinates in the o-file (tc-AFM-o.txt) and use them to plot your diagrams.

Following the identical recipe we can calculate the coordinates for the assemblage of chloritoid–chlorite–biotite at the same P – T (I’m skipping a few steps as they are the same as previously):

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

```

-----
P (kbar)      T (C)      x (mu)      y (mu)      x (bi)      y (bi)      Q (bi)      x (chl)
10.0000      530.000      0.7753      0.8494      0.8957      0.09136      0.03977      0.8520
              y (chl)    QAl (chl)    Q1 (chl)    Q4 (chl)    x (ctd)
              0.6008      0.3991      0.06058      0.1280      0.9614

proj          a          f          m          q          H2O          mu          phase
bi            -0.3790      1.2442      0.1348      -0.1210                                0.5000      -0.5000
chl           0.2003      0.6814      0.1184      0.4664      0.6667                                -0.1667

```


ctd	0.5000	0.4807	0.0193	0.5000	0.5000	-0.5000
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As well as the assemblages for the kyanite + chloritoid \rightarrow staurolite + chlorite reaction, starting with chlorite–chloritoid–kyanite:

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

P (kbar)	T (C)	x (mu)	y (mu)	x (chl)	y (chl)	QAl (chl)	Ql (chl)
10.0000	530.000	0.3303	0.9199	0.3171	0.7202	0.2796	0.03386
		Q4 (chl)	x (ctd)				
		0.04445	0.7297				
proj	a	f	m	q	H2O	mu	phase
chl	0.2401	0.2409	0.5190	0.4266	0.6667		-0.1667
ctd	0.5000	0.3649	0.1351	0.5000	0.5000		-0.5000
ky	1.0000			1.0000			-1.0000

Finally, the assemblage of staurolite–chloritoid–kyanite at 10 kbar & 530 °C:

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

2<== nothing in range ==>

This output suggests that one or several of the reacting minerals reached an end-member composition and terminated in a subsystem, meaning the assemblage cannot be represented on the AFM plane. We have encountered a similar situation when calculating the P – T projection in the previous tutorial. Finally, we explore higher variance assemblages such as chloritoid–chlorite:

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

```
-----
P (kbar)      T (C)      x (mu)      y (mu)      x (chl)      y (chl)      QAl (chl)      Ql (chl)
10.0000      530.000      0.4401      0.8946      0.4629      0.6555      0.3444      0.07853
              Q4 (chl)      x (ctd)
              0.08898      0.8289

mode          mu          chl          ctd          q          H2O      (note these)
              0.3097      0.08894      0.2239      0.3398      0.03769

proj          a          f          m          q          H2O          mu          phase
chl          0.2185      0.3618      0.4198      0.4482      0.6667          -0.1667
ctd          0.5000      0.4145      0.0855      0.5000      0.5000          -0.5000

comp          a          f          m          q          H2O          mu          bulk      (and these)
              0.4153      0.3986      0.1861      2.7829      0.8051      0.2993      -0.0642
```

Aha! THERMOCALC now also gives us the coordinates of the bulk composition we specified in the scriptfile. Why did we not get this result earlier you ask? This is because unlike the other assemblages we calculated so far, this one is actually 'seen' by the chosen bulk composition. Also, in this case THERMOCALC calculates the modal abundances of each mineral.

To calculate details of trivariant fields like chlorite + chloritoid, and therefore also the shape of the quadrivariant one-phase fields (specifically chlorite), you switch off pseudosection (i.e. “pseudosection no”), and rerun. Then THERMOCALC says:

you will have to set at least 1 compositional variable

specification of xyz isopleths

set compositional variables, from:x(mu) y(mu) x(chl) y(chl) QAl(chl) Q1(chl) Q4(chl) x(ctd)

which to set : x(ctd)

specifying isopleths for x(ctd):

low, high, inc OR one value : 0.05 0.45 0.1

x(ctd) set to values between 0.05 and 0.45

and the calculation gives

<=====>

phases: chl ctd (mu, q, fluid)

P (kbar)	T (C)	x(mu)	y(mu)	x(chl)	y(chl)	QAl(chl)	Q1(chl)	Q4(chl)	x(ctd)
10.000	530.00	0.02125	0.9790	0.01453	0.9140	0.08552	-0.006704	-0.001693	0.05

(note that the successive calculations involve x(ctd) increments)

proj	a	f	m	q	H2O	mu	phase
chl	0.3047	0.0101	0.6852	0.3620	0.6667		-0.1667
ctd	0.5000	0.0250	0.4750	0.5000	0.5000		-0.5000

```

-----
P (kbar)      T (C)      x (mu)      y (mu)      x (chl)      y (chl)      QAl (chl)      Q1 (chl)      Q4 (chl)      x (ctd)
10.000      530.00      0.06065      0.9749      0.04336      0.9021      0.09751      -0.01638      -0.003392      0.15

proj          a          f          m          q          H2O          mu          phase
chl          0.3007      0.0303      0.6690      0.3660      0.6667          -0.1667
ctd          0.5000      0.0750      0.4250      0.5000      0.5000          -0.5000
-----

P (kbar)      T (C)      x (mu)      y (mu)      x (chl)      y (chl)      QAl (chl)      Q1 (chl)      Q4 (chl)      x (ctd)
10.000      530.00      0.09763      0.9700      0.07282      0.8880      0.1116      -0.02182      -0.003123      0.25

proj          a          f          m          q          H2O          mu          phase
chl          0.2960      0.0513      0.6527      0.3707      0.6667          -0.1667
ctd          0.5000      0.1250      0.3750      0.5000      0.5000          -0.5000
-----

...

```

The finished AFM diagram for 10 kbar & 530 °C looks something like this:

You can now calculate your own AFM plots at any P - T conditions!

