

The “background>introduction” and “background>calculating mineral equilibria” sections provide a necessary introduction to this section. We shall assume that an appropriate THERMOCALC datafile has already been made for the model system of interest.

*PT* projections show the stable univariant and invariant equilibria for all of the composition space of the model system. Depending on whether univariants affect parts of the composition space that are petrologically interesting, *PT* projections may not be very interesting in themselves. Given that the compositions of the phases vary along univariants in *PT* projections, sometimes quickly, the parts of composition space that are affected by univariants may be difficult to gauge. With the exception of simple systems, *PT* projections can be almost impossible to use directly.

Pseudosections show the dependence of phase relationships of particular model system compositions on *PT*, so can be used to relate how particular rocks respond to changing metamorphic conditions. As a consequence they are often the most important phase diagrams to draw. Our interest in drawing *PT* projections is often only as an essential precursor to drawing pseudosections.

Compatibility diagrams show all the phase relationships for all compositions in the model system at the specified *PT*. As choosing phases to be “in excess” to reduce the model system to being effectively ternary—so that a triangular compatibility diagram can be drawn—may be difficult or impossible for the larger systems now being considered, compatibility diagrams are becoming less important.

## Calculating *PT* projections

The constructional features of *P–T* projections, involving invariant<sup>1</sup> points and univariant lines, are generally familiar.

Getting THERMOCALC to calculate the lines and points for a *P–T* projection is simple a matter of specifying the phases involved, and the variance of the equilibria required. Generally it is best to do this with the phases for each invariant point in turn, calculating the position of the invariant point, and all the univariants around the point. Schreinemaker analysis at each point is then done, followed by the putting together of the invariant points to determine which are stable.

Depending on the model system, there be many or a very few stable invariant points. In NCFMASH for blueschists and eclogites there are over a hundred (ask Gisella Rebay who has calculated them!), whereas in NCKFMASH at upper amphibolite and granulite facies conditions there are only a few univariants and one invariant (see White *et al.* 2001). Nevertheless knowing the *PT* projection is a necessary step because it provides the overall stability framework of the phase equilibria, and, if any univariants are stable in the pseudosection, this gives an invaluable start to the construction of the pseudosection.

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<sup>1</sup>for an  $n$  component system, involving  $p$  phases, the variance  $v$  is equal to  $n - p + 2$ , otherwise known as the phase rule. Invariant:  $v = 0$ ; univariant:  $v = 1$ ; divariant:  $v = 2$ ; and so on

The annotated log files in the old web site (*circa* Powell *et al.*, 1998) are a good place to look at this point (although things have changed a little bit since then). The simplicity of calculating an invariant (with TH KA1, a datafile with coding of the minerals in KFMASH<sup>2</sup>) can be seen from the following log file—user input is highlighted. An ellipsis at the end of a line signals that some output has been cut out. Where it says “(from script)”, it means that the action was controlled by a datafile script; where it says “(nothing input)”, it means that on the prompt for information return was hit, resulting in a default being used (in the case here, the *PT* window comes from the “setdefTwindow” and “setdefPwindow” scripts in the datafile).

```

reading phase info from this file ...
chl bi cd st ctd g mu ksp ky sill and q H2O
which phases : bi st g chl ky
fluid in excess (from script)
phases in excess: mu q (from script)

variance of required equilibria :
    0 = invariant
    1 = univariant
    2 = divariant
    ...
    n = n-variant
variance : 0

specification of PT window:
PT window within which invariant points expected to lie
T low,high, P low,high : (nothing input)

<=====>
phases : chl, bi, st, g, ky, (mu, q, fluid)
reactions : |XXXX|XX|XXX|XX|--X
P(kbar)      T(C)    x(chl)    y(chl)    Q(chl)    x(bi)    y(bi)    Q(bi)    x(st)    x(g) ...
  11.20     639.6   0.3067   0.5534   0.4465   0.3495   0.2008   0.4348   0.7462   0.7244 ...

```

Note that output gives the composition of all the phases at the invariant as well as its *PT*. (It also gives the state of order of the chlorite and muscovite—the *Q* values). Compared to the figures in Powell *et al.* (1998), this is a somewhat different result, being at about a kbar higher *P*, for several reasons: one is the more recent dataset used, the other is that chlorite and biotite are modelled using order-disorder. (Adding the script “calcsdnlc yes” to the datafile and rerunning shows that this *P* has a  $2\sigma$  uncertainty of about 1.5 kbar, so the difference is not considered to be a problem).

Running a univariant is almost as easy:

```

chl bi cd st ctd g mu ksp ky sill and q H2O
which phases : bi chl st g
fluid in excess (from script)
phases in excess: mu q (from script)

```

<sup>2</sup>the datafile name organisation is given in a separate documentation file

```

variance of required equilibria :
  0 = invariant
  1 = univariant
  2 = divariant
  ...
  n = n-variant
variance : 1

```

```

specification of PT window:
P range over which T of reactions to be calculated
P window: P low,high : 4 12
T window within which reactions expected to lie
T window: T low,high : (nothing input)
P window :4 <-> 16 kbar :P interval : 2

```

```

<=====>
phases : chl, bi, st, g, (mu, q, fluid)
reactions : |XXX|X|X|XXX|XX|-X
P(kbar)      T(C)    x(chl)    y(chl)    Q(chl)    x(bi)    y(bi)    Q(bi)    x(st)    x(g) ...
  4.00      536.2    0.8803    0.6724    0.3276    0.9293    0.6216    0.02812   0.9822   0.9816 ...
           22chl + 42g + 86mu = 86bi + 10st + 178q + 69H2O
  6.00      579.4    0.6017    0.5981    0.4018    0.6663    0.4169    0.2107    0.9155   0.9111 ...
           31chl + 23g + 74mu = 74bi + 10st + 125q + 103H2O
  8.00      606.5    0.4608    0.5742    0.4258    0.5022    0.2861    0.3649    0.8552   0.8458 ...
           33chl + 17g + 68mu = 68bi + 10st + 102q + 112H2O
 10.00      628.0    0.3586    0.5598    0.4401    0.3990    0.2237    0.4283    0.7900   0.7736 ...
           33chl + 16g + 66mu = 66bi + 10st + 96q + 111H2O
 12.00      646.9    0.2750    0.5498    0.4502    0.3191    0.1888    0.4289    0.7148   0.6887 ...
           32chl + 17g + 65mu = 65bi + 10st + 96q + 108H2O

```

The output gives the composition of the phases along the univariant as well as the  $T$  at each specified  $P$ . Note how the minerals change composition along the univariant, with  $x$  for the ferromagnesians becoming larger as  $P$  increases. The output also gives the balanced reaction (each mineral on on a one oxide basis) at each  $P$ .

Calculating along a stable univariant, 3 things can happen:

1. the univariant is cut off by a invariant, as happens in the above case with the invariant involving, additionally, kyanite (also calculated above). The relative stabilities have to be established with Schreinemakers analysis.
2. the univariant dies at an end-member system invariant, as would happen along the above calculated reaction at about 3.5 kbar, in the KFLASH system. It then remains to be established whether the univariant survives to that point, or is cut off by an invariant. In this case, the latter is true, with a full-system invariant involving, additionally, chloritoid (at 4.2 kbar).
3. THERMOCALC fails to calculate the univariant beyond a certain point, but no end-member system invariant is being approached. This signals a failure of the non-linear equation solver in THERMOCALC. The usual resolution is to vary the starting guesses in the datafile, using ones that correspond to the values along the univariant that THERMOCALC could calculate.

Later in this file, some special cases and special tricks are outlined.

## Calculating $PT$ and $Tx/Px$ pseudosections

Pseudosections involve the invariant and univariant equilibria they inherit from  $PT$  projections, as well as additional boundary lines and points. In a  $PT$  pseudosection these inherited equilibria are just those parts of the  $PT$  projection “seen” by the bulk composition being considered. In a  $Tx$  pseudosection these inherited equilibria occur as horizontal lines, spanning the range of bulk compositions that “sees” an equilibrium. The boundary lines and points separate fields of different variance; across lines the variance changes by one, and through points by two. The boundary points and lines can be most easily discussed with a new notation. Labelling is done in terms of the lower variance assemblage involved, with the names of phases with zero modes given in brackets. So for example in Fig. 1(iii), going from the g–chl–bi divariant field, through the point at 8 kbar and 580°C, into the chl quadrivariant field, the modes of bi and g both go to zero at the point. The point is therefore labelled “chl (bi g)”. Similarly, in going down  $T$  at 10 kbar from the g–chl–bi divariant field into the g–chl trivariant field into the chl quadrivariant field, the two lines crossed are labelled “chl g (bi)” and “chl (g)”.

The labelling of boundaries (and points) in terms of the phases whose mode(s) go to zero is shown in Figs 1 and 2. In THERMOCALC terminology such a boundary line is called “effectively” univariant (regardless of the variance of the fields) because, in terms of variables, the boundary is a line. The effective univariance<sup>3</sup> comes from the combining of the bulk composition with the equilibrium relationships.

In terms of a coherent view of pseudosection construction features, different rules appear to apply across univariants, with this being the one situation in which variance does not change by one (or, alternatively, the number of phase in the assemblage changing by one) across a “boundary”. In the (proper) univariant case, divariant fields occur across the univariant, with the swapping of (just) one phase in the assemblage. However, the univariant case can be made to comply with all others by representing the univariant as an (infinitely) thin field involving the full univariant assemblage. Then the standard way of thinking about boundaries in pseudosections applies to univariants as well.

Points in pseudosections are where two modes are zero with respect to the lowest variance assemblage at the point. At a point there is one  $n + 1$ , two  $n$ , and one  $n - 1$  variance fields. The two  $n - 1$  to  $n$  variance field boundaries involve one each of the phases whose modes are zero at the point. In terms of calculation, these two boundaries terminate at the point, whereas the other two boundaries ( $n$  to  $n + 1$  variance field boundaries) continue through the point. Considering a compatibility diagram, like the portion of AFM in (a) in Fig 3, and considering that the phase relations move with respect to the bulk composition (star) with changing  $PT$ , the variance relationships around points in  $PT$  pseudosections should be clear(er), as well as accounting for which lines will have metastable extensions.

Getting started in drawing a pseudosection is particularly straightforward if a univariant that is known to be stable (from the  $PT$  projection) is “seen” by the bulk composition (see below). Otherwise it is a matter of inspired guesswork, or Gibbs energy minimisation (via dogmin) can be used as a last resort.

Calculating along a line, 3 things can happen:

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<sup>3</sup>it is possible that there will be an argument over whether this is a traducing of the variance idea, but I think not, in terms of number of equations and number of variables, *once* a bulk composition is specified. . .

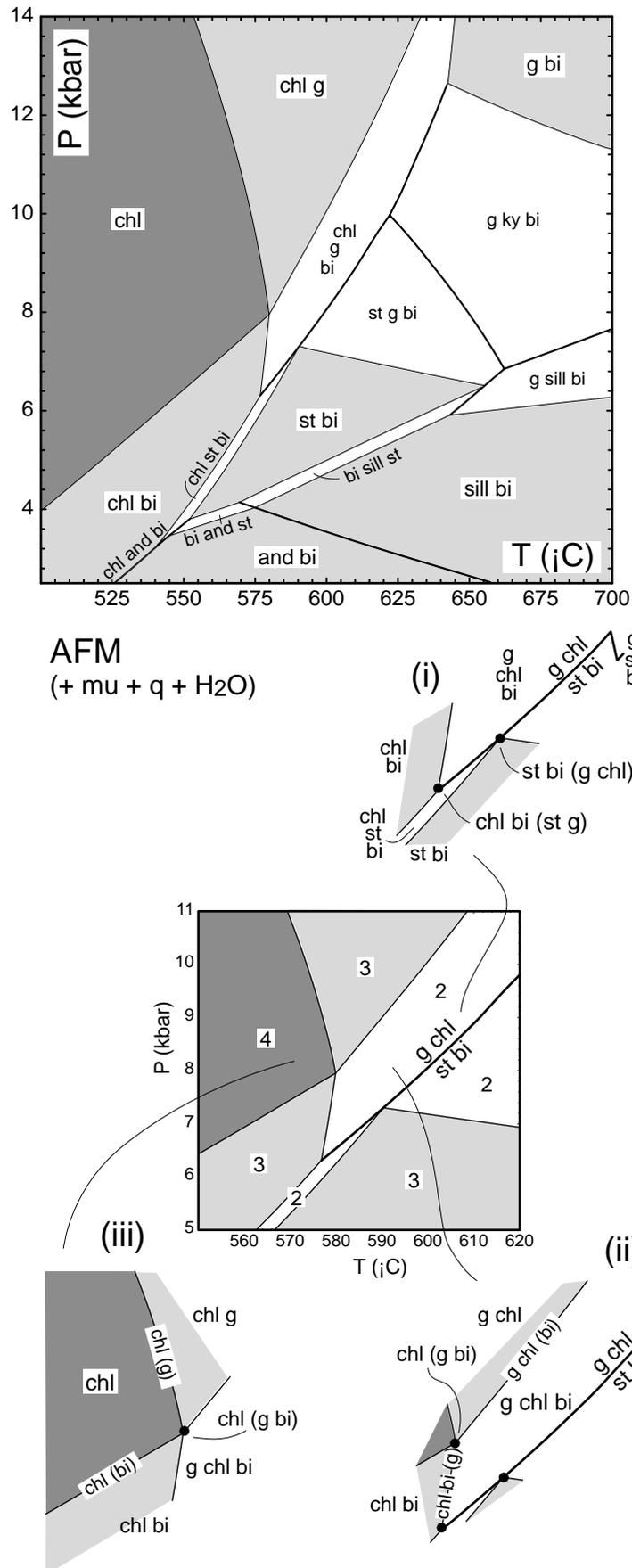


Fig. 1. The constructional features of part of the PT pseudosection in the top figure, indicating the necessary calculations to define the lines and points. The numbers give the variance of the corresponding field. In parts (i-iii), points and lines are labelled in terms of the lower variance adjacent assemblage, with the phase(s) whose modes are zero there being given in brackets. Part (i) focusses on the  $g + chl = st + bi$  univariant line, showing its relationship to adjoining trivariant fields that terminate on it; (ii) focusses on the  $g - chl - bi$  divariant field, its boundary lines at higher P being with trivariant fields, whereas the lower P boundary is the univariant; and (iii) focusses on the chl quadrivariant field.

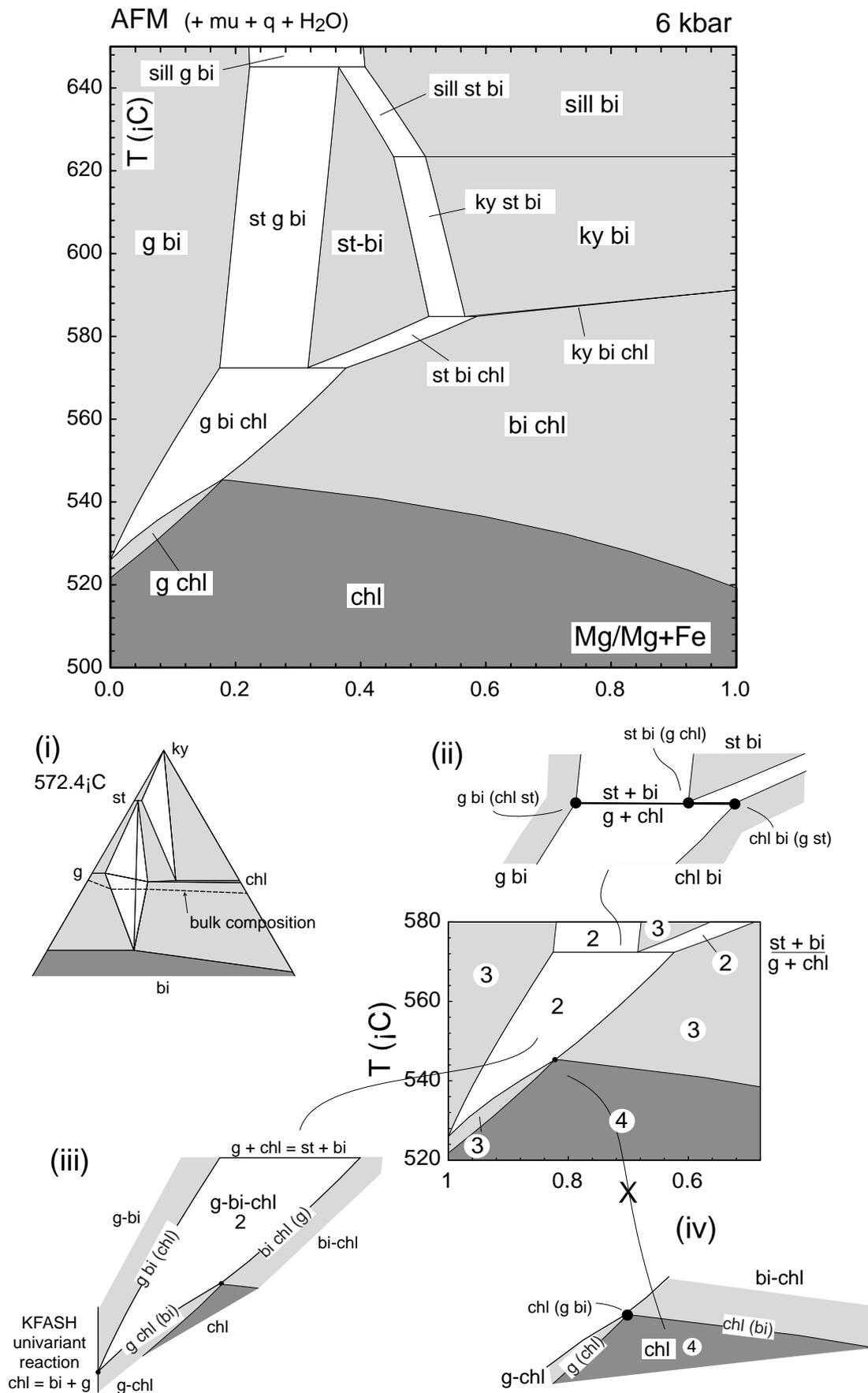
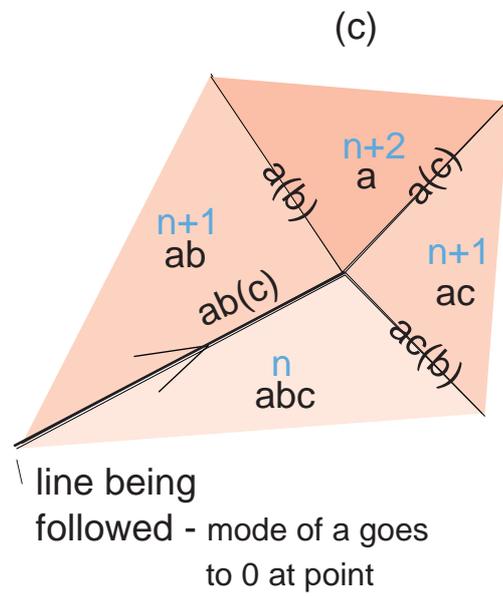
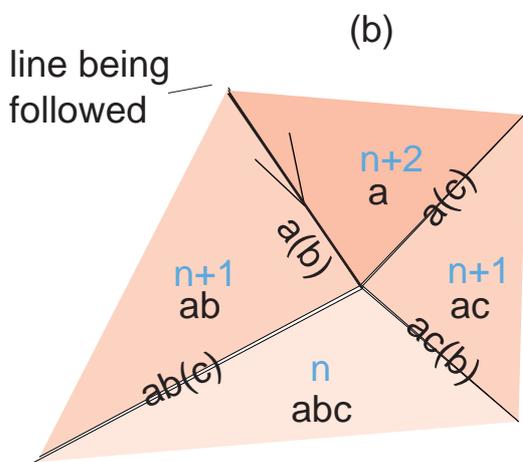
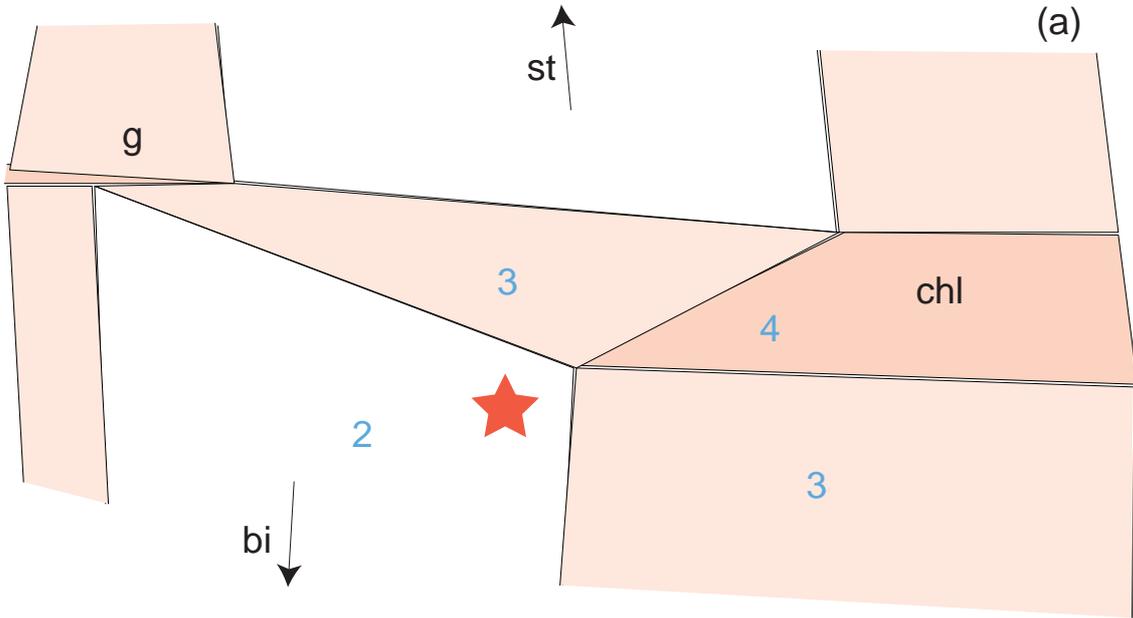


Fig. 2. The constructive features of part of the T-x pseudosection in top figure. The numbers give the variance of the corresponding field. In parts (ii-iv), points and lines are labelled as in Fig. 1. Part (i) shows the AFM diagram at the temperature of the  $g + chl = st + bi$  univariant equilibrium, showing where the composition line of the T-x diagram plots at this temperature, in projection from the calculated compositions of muscovite; (ii) focusses on the  $g + chl = st + bi$  univariant line; (iii) focusses on the g-chl-bi divariant field; (iv) focusses on the chl quadrivariant field.



1. the line is cut off by a *lower* variance field, with a new phase joining the equilibrium. If this line is a boundary between an  $n$  and an  $n + 1$  variant fields, then at the point where the line is cut off, an  $n - 1$ , two  $n$  and an  $n + 1$  variant fields meet. Case (b) in Fig 3.
2. the line dies, with a mode going to zero. If this line is a boundary between an  $n$  and an  $n + 1$  variant fields, then at the point where the line is cut off, an  $n$ , two  $n + 1$  and an  $n + 2$  variant fields meet. Case (c) in the Fig 3.
3. THERMOCALC fails to calculate the line beyond a certain point, but no mode is going to zero. This signals a failure of the non-linear equation solver in THERMOCALC. The usual resolution is to vary the starting guesses in the datafile, using ones that correspond to the values along the univariant that THERMOCALC could calculate.

Calculating a point, 2 things can happen:

1. the point is calculated successfully.
2. THERMOCALC fails to calculate the point. This can arise for two reasons: 1. The qualitative assessment of the pseudosection geometry is flawed, and the point is not there to be found. This can easily happen locating where trivariants touch univariants, when a narrow field has been missed, for example. 2. A failure of the non-linear equation solver in THERMOCALC is signalled. As before, the usual resolution is to vary the starting guesses.

Calculating the part of a univariant that is “seen” is illustrated for our KFMASH example (using datafile TH DKA2):

```

chl bi cd st ctd g mu ksp ky sill and q H20
which phases : (bi st g chl)
fluid in excess (from script)
phases in excess: mu q (from script)

variance of required equilibria :
  0 = invariant
  1 = univariant
  2 = divariant
  ...
  n = n-variant
variance : (1)
you may set zero modal proportions, from:chl bi st g mu q H20
which to set : ((nothing input))
equilibria now effectively univariant (eg a line in PT)

specification of PT window:
P range over which T of reactions to be calculated
P window: P low,high : (6 8.5)
T window within which reactions expected to lie
T window: T low,high : ((nothing input))
P window :6 <-> 9 kbar :P interval : (0.5)

composition (from script)
Al2O3  MgO  FeO  K2O
41.89  18.19  27.29  12.63

```

```

<=====>
phases : chl, bi, st, g, (mu, q, fluid)
reactions : |XXX|X|X|XXX|XX|-X
P(kbar)      T(C)    x(chl)  y(chl)  Q(chl)  x(bi)  y(bi)  Q(bi)  x(st)  x(g)...
  6.00      579.4   0.6017  0.5981  0.4018  0.6663  0.4169  0.2107  0.9155  0.9111...
      31chl + 23g + 74mu = 74bi + 10st + 125q + 103H2O
  6.50      587.0   0.5602  0.5905  0.4095  0.6163  0.3747  0.2582  0.9005  0.8949..
      32chl + 20g + 72mu = 72bi + 10st + 116q + 108H2O

mode      chl      bi      st      g      mu
  0.8709  0.1043          0.0248  0.4751
  0.7708  0.1916  0.0376          0.4477
-----
P(kbar)      T(C)    x(chl)  y(chl)  Q(chl)  x(bi)  y(bi)  Q(bi)  x(st)  x(g)...
  7.00      594.0   0.5238  0.5842  0.4158  0.5730  0.3392  0.3002  0.8855  0.8788...
      33chl + 19g + 70mu = 70bi + 10st + 110q + 110H2O

mode      chl      bi      st      g      mu
  0.7660  0.1138          0.1202  0.4730
  0.3187  0.5079  0.1734          0.3333
-----
P(kbar)      T(C)    x(chl)  y(chl)  Q(chl)  x(bi)  y(bi)  Q(bi)  x(st)  x(g)...
  7.50      600.4   0.4909  0.5788  0.4211  0.5353  0.3101  0.3357  0.8705  0.8625...
      33chl + 17g + 69mu = 69bi + 10st + 105q + 112H2O

mode      chl      bi      st      g      mu
  0.6780  0.1212          0.2008  0.4715
      0.7258  0.2707  0.0035  0.2362
-----
P(kbar)      T(C)    x(chl)  y(chl)  Q(chl)  x(bi)  y(bi)  Q(bi)  x(st)  x(g)...
  8.00      606.5   0.4608  0.5742  0.4258  0.5022  0.2861  0.3649  0.8552  0.8458...
      33chl + 17g + 68mu = 68bi + 10st + 102q + 112H2O

mode      chl      bi      st      g      mu
  0.6010  0.1274          0.2716  0.4703
      0.6711  0.2468  0.0821  0.2683
-----
P(kbar)      T(C)    x(chl)  y(chl)  Q(chl)  x(bi)  y(bi)  Q(bi)  x(st)  x(g)...
  8.50      612.2   0.4329  0.5700  0.4299  0.4728  0.2663  0.3881  0.8396  0.8287...
      33chl + 16g + 67mu = 67bi + 10st + 100q + 112H2O

mode      chl      bi      st      g      mu
  0.5310  0.1329          0.3361  0.4693
      0.6216  0.2242  0.1542  0.2950

```

---

Looking at this output, no mode output is given for 6 kbar, but is for 6.5 kbar, signalling that the “seen” part of the univariant starts between these pressures. The two lines of mode information relate to the two sides of the reaction: across univariants is the *one* place in pseudosections that modes change discontinuously. Looking down pressure through the mode information, the modes of garnet and staurolite are both going to zero towards the end point of the univariant (so the point is **bi chl (g st)**). Looking at the high *T* side of the reaction, there is a change in the assemblage, signalling that the **st + bi** trivariant touches the univariant here (the point being **st bi (g chl)**). These points are easy to calculate, for example:

---

```

chl bi cd st ctd g mu ksp ky sill and q H2O
which phases : (bi st g chl)
fluid in excess (from script)
phases in excess: mu q (from script)

variance of required equilibria :
  0 = invariant
  1 = univariant
  2 = divariant
  ...
  n = n-variant
variance : (1)
you may set zero modal proportions, from:chl bi st g mu q H2O
which to set : (g st)
equilibria now effectively invariant (eg a point in PT)

```

```

specification of PT window:
PT window within which invariant points expected to lie
T low,high, P low,high : (nothing input)

```

```

composition (from script)
Al2O3 MgO FeO K2O
41.89 18.19 27.29 12.63
<=====>
phases : chl, bi, st, g, (mu, q, fluid)
reactions : |XXX|X|X|XXX|XX|-X

```

---

P(kbar)	T(C)	x(chl)	y(chl)	Q(chl)	x(bi)	y(bi)	Q(bi)	x(st)	x(g)...
6.39	585.3	0.5692	0.5921	0.4078	0.6271	0.3838	0.2477	0.9039	0.8986...
mode	chl	bi	st	g	mu				
	0.3858	0.04366	0	0	0.5705				

---

Now, the g + chl + bi divariant on the low temperature side of the univariant goes into the chl + bi trivariant at the low pressure end of the “seen” part of the univariant, so there is the bi chl (g) line to calculate. So

---

```

chl bi cd st ctd g mu ksp ky sill and q H2O
which phases : (bi chl g)
fluid in excess (from script)
phases in excess: mu q (from script)

variance of required equilibria :
  0 = invariant
  1 = univariant
  2 = divariant
  ...
  n = n-variant
variance : (2)

```

you may set zero modal proportions, from:chl bi g mu q H2O  
 which to set : **g**  
 equilibria now effectively univariant (eg a line in PT)

specification of PT window:  
 P range over which T of reactions to be calculated  
 P window: P low,high : **6 9**  
 T window within which reactions expected to lie  
 T window: T low,high : (nothing input)  
 P window :6 <-> 9 kbar :P interval : **0.5**

composition (from script)  
 Al2O3 MgO FeO K2O  
 41.89 18.19 27.29 12.63  
 <=====>  
 phases : chl, bi, g, (mu, q, fluid)  
 reactions : |XX|X|XXX|XX|-X

P(kbar)	T(C)	x(chl)	y(chl)	Q(chl)	x(bi)	y(bi)	Q(bi)	x(g)...
6.00	584.9	0.5687	0.6054	0.3945	0.6335	0.4219	0.2257	0.8981...
mode	chl	bi	g	mu				
	0.3769	0.06536	0	0.5577				
P(kbar)	T(C)	x(chl)	y(chl)	Q(chl)	x(bi)	y(bi)	Q(bi)	x(g)...
6.50	585.4	0.5692	0.5887	0.4113	0.6251	0.3727	0.2543	0.8987...
mode	chl	bi	g	mu				
	0.3882	0.03771	0	0.5741				
P(kbar)	T(C)	x(chl)	y(chl)	Q(chl)	x(bi)	y(bi)	Q(bi)	x(g)...
7.00	586.0	0.5686	0.5758	0.4241	0.6160	0.3272	0.2829	0.8986...
mode	chl	bi	g	mu				
	0.3977	0.01402	0	0.5882				

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Along this line to higher pressure, the mode of biotite is going to zero, signalling case (c) in Fig. 3. And so on. In this way a pseudosection is built up line-by-line and point-by-point.

## Calculating compatibility diagrams

The constructional features of compatibility diagrams are illustrated in Fig. 4. The tie triangles (divariant equilibria) in the full system (within the triangle) as well as the divariant equilibria in the subsystems (edges of the triangle) specify much of the geometry, including the apices of the one-phase fields (quadrivariant equilibria). The edges of the one phase fields can be determined via the adjacent trivariant equilibria. In cases such as this, in which Fe–Mg is the dominant substitution, the edges are close to being straight; in other systems, such edges can be strongly curved. For example, running a divariant:

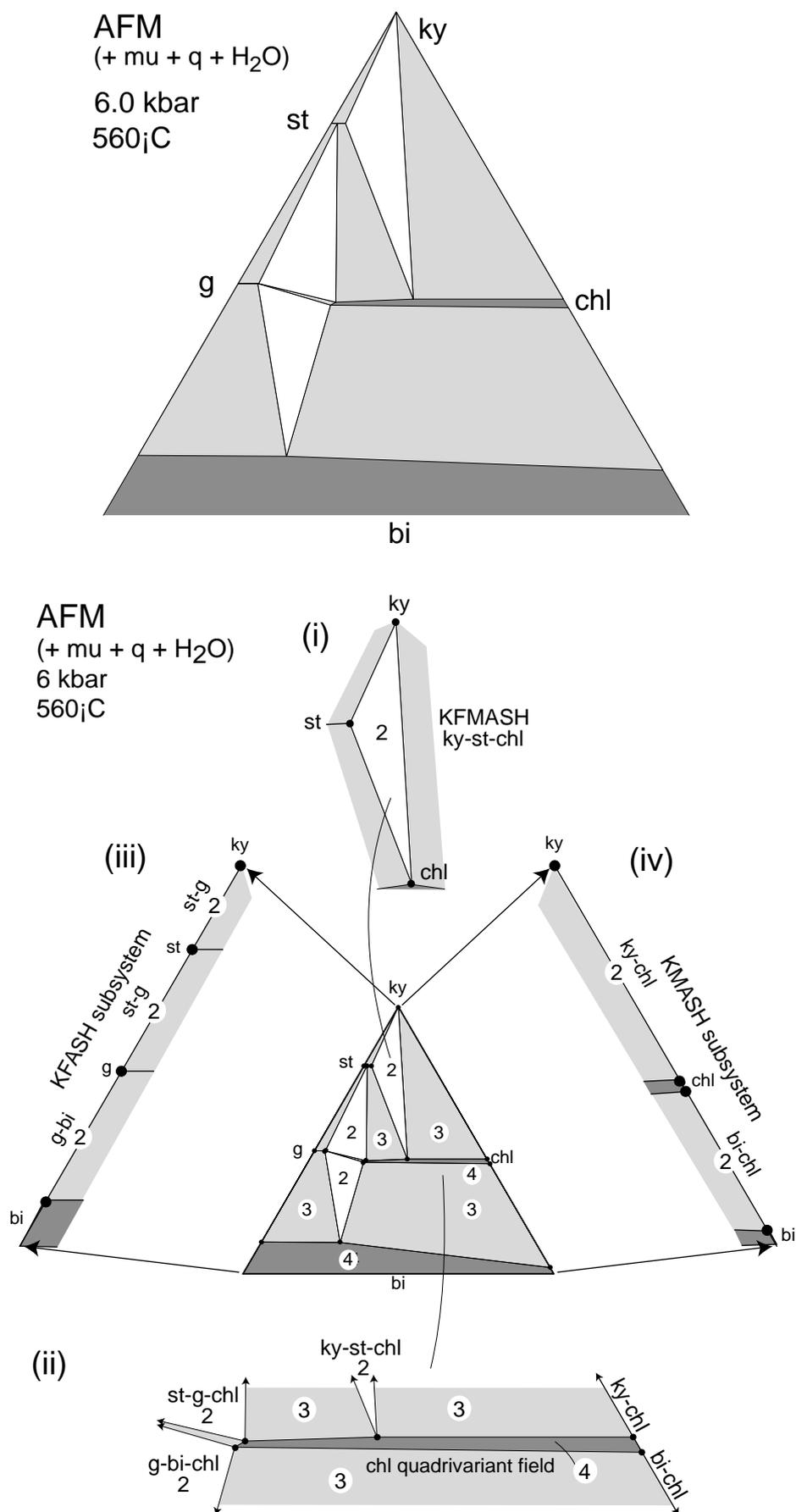


Fig. 3. The constructional features of the AFM compatibility diagram in the top figure. The numbers give the variance of the corresponding field. Part (i) focusses on a full-system divariant field; (ii) focusses on the chlorite one-phase field; its apices are defined by the corresponding apices of the full and subsystem divariant fields; (iii) focusses on the KFASH divariant fields that define the left hand edge of the diagram, (iv), focusses on the KMASH divariant fields on the right edge

---

```
chl bi cd st ctd g mu ksp ky sill and q H2O
which phases : (bi g chl)
fluid in excess (from script)
phases in excess: mu q (from script)
```

```
variance of required equilibria :
  0 = invariant
  1 = univariant
  2 = divariant
  3 = trivariant
  ...
  n = n-variant
variance : (2)
```

```
specification of PT window:
P range over which equilibria to be calculated
P window: P low,high : (8)
T range over which equilibria to be calculated
T window: T low,high : (600)
```

```
projection plane has 3 apices, leaving Al2O3 MgO FeO K2O
to be represented by mu and the projection plane
projection plane (from script)
```

	Al2O3	MgO	FeO	K2O
A	1.000	0	0	0
F	0	0	1.000	0
M	0	1.000	0	0

```
<=====>
phases : chl, bi, g, (mu, q, fluid)
reactions : |XX|X|XXX|XX|-X
```

---

P(kbar)	T(C)	x(chl)	y(chl)	Q(chl)	x(bi)	y(bi)	Q(bi)	x(g)...
8.00	600.0	0.4929	0.5682	0.4317	0.5313	0.2726	0.3606	0.8639...

proj	A	F	M	mu	phase
chl	0.189	0.400	0.411		-0.167
bi	-0.261	0.643	0.618	0.500	-0.500
g	0.250	0.648	0.102		-0.250

---

The output gives the coordinates in the AFM triangle, the projection being from the *calculated* composition of muscovite, as well as quartz and H<sub>2</sub>O.

## Special cases and tricks-of-the-trade

1. In calculating univariants in *PT* projections, strongly curved ones and ones along which the phase change composition quickly can be awkward to calculate. One way to do this is to use isopleths (via the script "setiso"). If a phases composition, eg x(chl), changes progressively along the univariant, the univariant can be calculated as a series of effectively invariant points, each with a fixed value of x(chl). Running with TH DKA1A:

---

chl bi cd st ctd g mu ksp ky sill and q H2O  
 which phases : chl st g bi  
 fluid in excess (from script)  
 phases in excess: mu q (from script)

variance of required equilibria :  
 0 = invariant  
 1 = univariant  
 2 = divariant  
 ...  
 n = n-variant

variance : 1

you may set compositional variables, from:

x(chl) y(chl) Q(chl) x(bi) y(bi) Q(bi) x(st) x(g) x(mu) y(mu)  
 (maximum number to set = 1)  
 which variables to set : x(chl)

how to specify isopleth for x(chl):

0: list of values  
 1: start, finish, interval

code : 1

isopleth: low,high,interval : 0.3 0.9 0.1

equilibria now effectively invariant (eg a point in PT)

specification of PT window:

PT window within which invariant points expected to lie  
 T low,high, P low,high : (nothing input)

<=====>

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

reactions : |XXX|X|X|XXX|XX|-X

P(kbar)	T(C)	x(chl)	y(chl)	Q(chl)	x(bi)	y(bi)	Q(bi)	x(st)...	
11.37	641.1	0.3	0.5526	0.4473	0.3431	0.1981	0.4342	0.7399...	
			32chl + 17g + 65mu = 65bi + 10st + 96q + 109H2O						
9.13	619.1	0.4	0.5654	0.4346	0.4394	0.2457	0.4100	0.8193...	
			33chl + 16g + 66mu = 66bi + 10st + 98q + 112H2O						
7.36	598.6	0.5	0.5803	0.4197	0.5456	0.3178	0.3262	0.8748...	
			33chl + 18g + 69mu = 69bi + 10st + 106q + 111H2O						
6.02	579.7	0.6	0.5978	0.4021	0.6642	0.4152	0.2126	0.9149...	
			31chl + 23g + 74mu = 74bi + 10st + 124q + 104H2O						
5.07	562.5	0.7	0.6189	0.3810	0.7776	0.5100	0.1176	0.9447.	
			28chl + 31g + 79mu = 79bi + 10st + 147q + 90H2O						
4.40	547.2	0.8	0.6455	0.3544	0.8700	0.5806	0.05805	0.9675...	
			24chl + 38g + 83mu = 83bi + 10st + 166q + 77H2O						
3.91	533.7	0.9	0.6797	0.3202	0.9422	0.6300	0.02240	0.9854...	
			22chl + 43g + 86mu = 86bi + 10st + 180q + 67H2O						

---

2. Watch out for singularities, where phases change sides on reactions, along a reaction's length. Unless these are recognised, and they can be arbitrarily close to invariants, they can make a mess of the Schreinemakers analysis.

3. THERMOCALC does *not* tell which way around univariant reactions are. It makes a guess, but does not always get it right. (This is high up on my list of things to code. It is actually a non-trivial problem.)
4. Degenerate univariant equilibria, like  $law = cz + ky + q + H_2O$  in NCFMASH, will be 'seen' by all lawsonite-bearing fields, regardless of their variance. Nevertheless, a divariant field that runs into this reaction will terminate in a *full* system univariant that can be calculated as such by THERMOCALC.

**top**

**back**