

Introductory T-x pseudosection tutorial

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This tutorial covers the basics for calculating a T-x pseudosection. Before doing this tutorial you should do the base level P-T pseudosection tutorial, much of the basic information regarding doing calculations is covered there and the diagram done here is based on that one.

What I will mostly cover in detail in this tutorial is those aspects of using THERMOCALC that are particular to T-x or P-x pseudosections.

This tutorial covers the construction of a T-x(Al) pseudosection where $x(\text{Al}) = \text{Al}_2\text{O}_3 / (\text{Al}_2\text{O}_3 + \text{FeO} + \text{MgO})$ where the XFe ($\text{FeO} / (\text{FeO} + \text{MgO})$) is kept constant. In terms of the main changes that will occur, this is equivalent to tracking up through an AFM triangle towards the 'A' apex. Considering what the equilibria must look like from a basic knowledge of the AFM compatibility diagram is useful for being able to predict when new phases may come in (though in some systems these diagrams are less useful).

This tutorial was prepared using THERMOCALC 3.30 and drawpd 1.11 (files for thermocalc 3.33 and drawpd 1.15 are given in a separate folder)
In your THERMOCALC folder you will need the following files

tc-tpstute
tc-NCKFMASHp
dr dtx1 (mac) or drdtx1 (pc) (or wherever you keep drawpd)

in addition a completed drawpd file (dr dtx1f or drdtx1f) and the postscript file from running this are included in the download

In your tc-prefs file use the scripts
calcmode 1
scriptfile tpstute

so THERMOCALC automatically uses this script file and knows you are doing phase diagram calculations.

The two endmember rock compositions I am using (normalized to 100% with some adjustment of the H₂O contents in addition to Al₂O₃) are shown below (look in the scripts file 'tpstute')

```
% -----  
%          H2O    SiO2   Al2O3   CaO    MgO    FeO    K2O    Na2O  
setbulk yes  6.03  70.44   7.06   0.27   3.66   8.97   2.99   0.58    % x=0  
setbulk yes  4.97  63.60  16.57   0.25   3.30   8.10   2.70   0.51    % x= 1  
% -----
```

In addition the script

```
setdefPwindow yes 5 5
```

means that the calculations will be done at 5 kbar if you hit return when prompted for a P range. Alternatively you could use the script

```
setPwindow yes 5 5
```

to automatically use 5 kbar, but this makes calculating points difficult.

In the dr dtxpstute file there are some features that are different than for a P-T pseudo. Firstly each line and point has 3 columns (x, P, T), so at the top of the file the scripts should read

```
3 % no of variables in each line of data,  
  % in this case, P, T  
  
5 % 6 (KFMASH) - 3 (+q+mu+H2O)  
  
1 3 % which columns to be x,y in phase diagram  
  
x 2 5 % x keyword turns on interpolation for points,  
      % involving column 2 at value 5 (kbar)
```

The highlighted text allows drawpd to interpolate where points will occur in T-x space at 5 kbar. This is all explained below.

The scripts at the bottom of the file look like:

```
window 0 1 700 860 % T,P window  
  
bigticks 0.1 0 50 700 % main T ticks at 20° intervals, starting at 500  
                % main P ticks at 1 kbar intervals, starting at 2  
  
smallticks 0.01 10 % minor T,P ticks  
  
darkcolour 58 0 127 % red green blue in 0<->255 => Illustrator RGB  
                % this choice gives the diagram in blues  
  
numbering yes
```

so x is the x-axis and T is the y-axis.

Run THERMOCALC, and you will be prompted by the which 'phases?' prompt. As the two bulk compositions used are a simple modification of that used in the P-T pseudosection tutorial, we can assume that each of the mineral assemblage field boundaries encountered in that diagram

at 5 kbar will be seen somewhere across our diagram. Going up T the first line encountered is the (g) line from the g-sill-bi-ksp-pl-q-liq trivariant field. So we can calculate that.

```
reading a-x datafile, "tc-NCKFMASHp.txt"...
ged anth bi cd st ctd chl g sp mu pa opx liq ksp pl osm
ky sill and q H2O
choose from: ged anth bi cd st ctd chl g sp mu pa opx liq ksp pl osm ky sill and q H2O
which phases : g sill bi ksp pl q liq
no phases in excess (from script)
```

variance of required equilibria :

```
0 = invariant
1 = univariant
2 = divariant
...
n = n-variant
```

variance : 3

you may set zero modal proportions, from:bi g liq ksp pl sill q

which to set : g

specification of PT window:

P range over which T of reactions to be calculated

P window: P low,high :

T window within which reactions expected to lie

T window: T low,high :

making a bulk composition range within the range specified,

start and finish proportions across bulk composition range : 0 1

how many increments (max = 100) : 25

Here I just hit return for the P window (ie 5 kbar). The two bulk compositions are read by THERMOCALC as position value 0 and value 1 respectively, so typing 0 1 when prompted by the start and finish proportions across bulk composition range, runs the calculation between the whole range of composition between the two bulks. The number of increments is simply the number of steps across the range chosen. In this example I set 25. The output should look something like (only the first few and last few lines shown):

composition

```
H2O SiO2 Al2O3 CaO MgO FeO K2O Na2O
6.03 70.44 7.06 0.27 3.66 8.97 2.99 0.58
4.97 63.60 16.57 0.25 3.30 8.10 2.70 0.51
```

(25 increments across 0 to 1.000 of original range)

<=====>

phases : bi, g, liq, ksp, pl, sill, q

| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(g) | z(g) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) | ca(pl) | k(pl) |
|---------|--------|--------|---------|---------|---------|----------|--------|--------|--------|----------|----------|--------|--------|---------|---------|--------|---------|
| 5.00 | 731.1 | 0.7101 | 0.5661 | 0.06370 | 0.8563 | 0.01718 | 0.1629 | 0.3024 | 0.5130 | 0.005928 | 0.002555 | 0.8208 | 0.5113 | 0.2818 | 0.01089 | 0.2494 | 0.05493 |
| mode | bi | g | liq | ksp | pl | sill | q | | | | | | | | | | |
| 0 | 0.3852 | 0 | 0.04077 | 0.02816 | 0.04050 | 0.004935 | 0.5004 | | | | | | | | | | |

| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(g) | z(g) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) | ca(pl) | k(pl) |
|---------|-------|--------|--------|---------|--------|---------|--------|--------|--------|----------|----------|--------|--------|---------|---------|--------|---------|
| 5.00 | 731.1 | 0.7101 | 0.5661 | 0.06370 | 0.8563 | 0.01716 | 0.1628 | 0.3024 | 0.5131 | 0.005922 | 0.002555 | 0.8208 | 0.5113 | 0.2820 | 0.01089 | 0.2490 | 0.05500 |

| mode | bi | g | liq | ksp | pl | sill | q |
|-------|--------|---|---------|---------|---------|---------|--------|
| 0.040 | 0.3838 | 0 | 0.03969 | 0.02836 | 0.04046 | 0.01309 | 0.4946 |

| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(g) | z(g) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) | ca(pl) | k(pl) |
|---------|-------|--------|--------|---------|--------|---------|--------|--------|--------|----------|----------|--------|--------|---------|---------|--------|---------|
| 5.00 | 731.1 | 0.7101 | 0.5661 | 0.06370 | 0.8563 | 0.01715 | 0.1628 | 0.3024 | 0.5133 | 0.005916 | 0.002554 | 0.8208 | 0.5114 | 0.2822 | 0.01089 | 0.2487 | 0.05506 |

| mode | bi | g | liq | ksp | pl | sill | q |
|-------|--------|---|---------|---------|---------|---------|--------|
| 0.080 | 0.3823 | 0 | 0.03862 | 0.02855 | 0.04043 | 0.02125 | 0.4889 |

.
. rest of the output here
.

| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(g) | z(g) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) | ca(pl) | k(pl) |
|---------|-------|--------|--------|---------|--------|---------|--------|--------|--------|----------|----------|--------|--------|---------|---------|--------|---------|
| 5.00 | 730.8 | 0.7105 | 0.5661 | 0.06363 | 0.8565 | 0.01678 | 0.1623 | 0.3027 | 0.5166 | 0.005773 | 0.002548 | 0.8210 | 0.5118 | 0.2864 | 0.01085 | 0.2408 | 0.05667 |

| mode | bi | g | liq | ksp | pl | sill | q |
|-------|--------|---|---------|---------|---------|--------|--------|
| 0.960 | 0.3495 | 0 | 0.01493 | 0.03282 | 0.03960 | 0.2008 | 0.3624 |

| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(g) | z(g) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) | ca(pl) | k(pl) |
|---------|-------|--------|--------|---------|--------|---------|--------|--------|--------|----------|----------|--------|--------|---------|---------|--------|---------|
| 5.00 | 730.7 | 0.7105 | 0.5661 | 0.06363 | 0.8565 | 0.01676 | 0.1623 | 0.3028 | 0.5168 | 0.005766 | 0.002547 | 0.8210 | 0.5118 | 0.2866 | 0.01085 | 0.2404 | 0.05674 |

| mode | bi | g | liq | ksp | pl | sill | q |
|-------|--------|---|---------|---------|---------|--------|--------|
| 1.000 | 0.3480 | 0 | 0.01385 | 0.03302 | 0.03957 | 0.2089 | 0.3566 |

so this line extends the whole way across the diagram unless it gets cut off by a lower variance assemblage.

The next line to calculate is the (cd) line from the g-cd-sill-bi-ksp-pl-q-liq divariant field. So entering this, setting v=2, setting cd to zero hitting return at the P range and T range prompts, calculating from 0 to 1 and setting 25 increments again

```
reading a-x datafile, "tc-NCKFMASHp.txt"...
ged anth bi cd st ctd chl g sp mu pa opx liq ksp pl osm
ky sill and q H2O
choose from: ged anth bi cd st ctd chl g sp mu pa opx liq ksp pl osm ky sill and q H2O
which phases : g sill bi ksp pl q liq
no phases in excess (from script)
```

variance of required equilibria :

```
0 = invariant
1 = univariant
2 = divariant
...
```

```
n = n-variant
```

variance : 2

you may set zero modal proportions, from:bi cd g liq ksp pl sill q

which to set : cd

specification of PT window:

P range over which T of reactions to be calculated

P window: P low,high :
T window within which reactions expected to lie
T window: T low,high :
making a bulk composition range within the range specified,
start and finish proportions across bulk composition range : 0 1
how many increments (max = 100) : 25

again, this equilibria can be calculated from 0 to 1

```
-----
P(kbar)    T(?C)    x(bi)    y(bi)    Q(bi)    x(cd)    h(cd)    x(g)    z(g)    q(L)    fsp(L)    na(L)    an(L)    ol(L)    x(L)    h2o(L)    na(ksp)    ca(ksp)    ca(pl)    k(pl)
  5.00      738.3    0.6830    0.5584    0.07075   0.4469   0.5988    0.8425   0.02096   0.1708   0.3005   0.4689   0.007853  0.002776   0.8099   0.5021   0.2364   0.01137   0.3465   0.04050

mode      bi      cd      g      liq      ksp      pl      sill      q
  0    0.3189      0    0.05068   0.08638   0.05948   0.02081  0.001181   0.4625
-----
.
.
.
-----
P(kbar)    T(?C)    x(bi)    y(bi)    Q(bi)    x(cd)    h(cd)    x(g)    z(g)    q(L)    fsp(L)    na(L)    an(L)    ol(L)    x(L)    h2o(L)    na(ksp)    ca(ksp)    ca(pl)    k(pl)
  5.00      737.9    0.6827    0.5582    0.07087   0.4466   0.5990    0.8424   0.02046   0.1700   0.3011   0.4742   0.007645  0.002770   0.8098   0.5025   0.2416   0.01136   0.3353   0.04192

mode      bi      cd      g      liq      ksp      pl      sill      q
1.000    0.2868      0    0.04684   0.05522   0.06281   0.02077   0.2055   0.3221
-----
```

so, the drawpd data from these two lines (in the tc-tpxstute-dr file) look like that below, and these two lines will be u1 & u2 and both go from begin to end.

```
% -----
u<k>    bi liq ksp pl sill q  - g

begin  end

0 5.00 731.1 % g = 0
0.0400 5.00 731.1 % g = 0
0.0800 5.00 731.1 % g = 0
0.1200 5.00 731.1 % g = 0
0.1600 5.00 731.1 % g = 0
0.2000 5.00 731.0 % g = 0
0.2400 5.00 731.0 % g = 0
0.2800 5.00 731.0 % g = 0
0.3200 5.00 731.0 % g = 0
0.3600 5.00 731.0 % g = 0
0.4000 5.00 731.0 % g = 0
0.4400 5.00 731.0 % g = 0
0.4800 5.00 730.9 % g = 0
0.5200 5.00 730.9 % g = 0
0.5600 5.00 730.9 % g = 0
0.6000 5.00 730.9 % g = 0
0.6400 5.00 730.9 % g = 0
0.6800 5.00 730.9 % g = 0
```

```

0.7200 5.00 730.8 % g = 0
0.7600 5.00 730.8 % g = 0
0.8000 5.00 730.8 % g = 0
0.8400 5.00 730.8 % g = 0
0.8800 5.00 730.8 % g = 0
0.9200 5.00 730.8 % g = 0
0.9600 5.00 730.8 % g = 0
1.0000 5.00 730.7 % g = 0

% -----
u<k>   bi g liq ksp pl sill q  - cd

begin  end

0 5.00 738.3 % cd = 0
0.0400 5.00 738.3 % cd = 0
0.0800 5.00 738.2 % cd = 0
0.1200 5.00 738.2 % cd = 0
0.1600 5.00 738.2 % cd = 0
0.2000 5.00 738.2 % cd = 0
0.2400 5.00 738.2 % cd = 0
0.2800 5.00 738.2 % cd = 0
0.3200 5.00 738.1 % cd = 0
0.3600 5.00 738.1 % cd = 0
0.4000 5.00 738.1 % cd = 0
0.4400 5.00 738.1 % cd = 0
0.4800 5.00 738.1 % cd = 0
0.5200 5.00 738.1 % cd = 0
0.5600 5.00 738.1 % cd = 0
0.6000 5.00 738.0 % cd = 0
0.6400 5.00 738.0 % cd = 0
0.6800 5.00 738.0 % cd = 0
0.7200 5.00 738.0 % cd = 0
0.7600 5.00 738.0 % cd = 0
0.8000 5.00 738.0 % cd = 0
0.8400 5.00 737.9 % cd = 0
0.8800 5.00 737.9 % cd = 0
0.9200 5.00 737.9 % cd = 0
0.9600 5.00 737.9 % cd = 0
1.0000 5.00 737.9 % cd = 0

```

The next line to be encountered in the P-T pseudosection from tute 1 is the (sill) line from the same divariant field. Again running from 0 to 1 and 25 increments gives:

```

-----
P(kbar)   T(?C)   x(bi)   y(bi)   Q(bi)   x(cd)   h(cd)   x(g)   z(g)   q(L)   fsp(L)   na(L)   an(L)   ol(L)   x(L)   h2o(L)   na(ks)   ca(ks)   ca(pl)   k(pl)
  5.00     738.5   0.6831  0.5585  0.07067  0.4471  0.5987  0.8426  0.02125  0.1712  0.3001  0.4658  0.007977  0.002779  0.8100  0.5018  0.2334  0.01137  0.3531  0.03970

mode      bi      cd      g      liq      ksp      pl      sill      q
  0   0.3145 0.003063 0.05267 0.08850 0.06165 0.01995  0      0.4597
-----
P(kbar)   T(?C)   x(bi)   y(bi)   Q(bi)   x(cd)   h(cd)   x(g)   z(g)   q(L)   fsp(L)   na(L)   an(L)   ol(L)   x(L)   h2o(L)   na(ks)   ca(ks)   ca(pl)   k(pl)
  5.00     740.1   0.6841  0.5593  0.07016  0.4486  0.5983  0.8433  0.02325  0.1744  0.2978  0.4439  0.008827  0.002802  0.8106  0.4998  0.2135  0.01137  0.3979  0.03485

```

| | | | | | | | | | | | | | | | | | | | | | |
|---------|--------|---------|---------|---------|---------|----------|--------|---------|--------|--------|--------|----------|----------|--------|--------|---------|---------|--------|---------|--|--|
| mode | bi | cd | g | liq | ksp | pl | sill | q | | | | | | | | | | | | | |
| 0.040 | 0.2821 | 0.02432 | 0.06630 | 0.1020 | 0.07614 | 0.01461 | 0 | 0.4345 | | | | | | | | | | | | | |
| ----- | | | | | | | | | | | | | | | | | | | | | |
| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(cd) | h(cd) | x(g) | z(g) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) | ca(pl) | k(pl) | | |
| 5.00 | 741.7 | 0.6852 | 0.5601 | 0.06965 | 0.4500 | 0.5979 | 0.8439 | 0.02519 | 0.1777 | 0.2953 | 0.4217 | 0.009671 | 0.002824 | 0.8112 | 0.4978 | 0.1953 | 0.01136 | 0.4411 | 0.03099 | | |
| ----- | | | | | | | | | | | | | | | | | | | | | |
| mode | bi | cd | g | liq | ksp | pl | sill | q | | | | | | | | | | | | | |
| 0.080 | 0.2496 | 0.04568 | 0.08002 | 0.1158 | 0.08974 | 0.01013 | 0 | 0.4091 | | | | | | | | | | | | | |
| ----- | | | | | | | | | | | | | | | | | | | | | |
| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(cd) | h(cd) | x(g) | z(g) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) | ca(pl) | k(pl) | | |
| 5.00 | 743.2 | 0.6864 | 0.5609 | 0.06915 | 0.4515 | 0.5976 | 0.8446 | 0.02702 | 0.1808 | 0.2930 | 0.3997 | 0.01049 | 0.002844 | 0.8117 | 0.4959 | 0.1789 | 0.01133 | 0.4814 | 0.02793 | | |
| ----- | | | | | | | | | | | | | | | | | | | | | |
| mode | bi | cd | g | liq | ksp | pl | sill | q | | | | | | | | | | | | | |
| 0.120 | 0.2169 | 0.06711 | 0.09388 | 0.1298 | 0.1027 | 0.006269 | 0 | 0.3834 | | | | | | | | | | | | | |
| ----- | | | | | | | | | | | | | | | | | | | | | |
| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(cd) | h(cd) | x(g) | z(g) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) | ca(pl) | k(pl) | | |
| 5.00 | 744.6 | 0.6874 | 0.5617 | 0.06867 | 0.4529 | 0.5973 | 0.8452 | 0.02873 | 0.1838 | 0.2907 | 0.3784 | 0.01126 | 0.002862 | 0.8123 | 0.4941 | 0.1644 | 0.01129 | 0.5184 | 0.02551 | | |
| ----- | | | | | | | | | | | | | | | | | | | | | |
| mode | bi | cd | g | liq | ksp | pl | sill | q | | | | | | | | | | | | | |
| 0.160 | 0.1839 | 0.08861 | 0.1079 | 0.1441 | 0.1153 | 0.002833 | 0 | 0.3574 | | | | | | | | | | | | | |

Thus, from looking at the modes this line terminates at a (sill pl) point.

Unlike with P-T pseudosections, points cannot be directly calculated in T-x or P-x pseudosections. There are three ways to define a point.

1) you could calculate all the lines around the point and use the 'crossover' code to define the point. The dr d code would look like

```
i1
crossover u3 u4
```

if you are defining the point via those two lines. This method does not always work and sometimes drawpd puts the point in an odd place.

2) you could run either of the low variance equilibria at very small increments and take as the point the data with, in this case, lowest mode of pl. i.e. you would re-run the last equilibria between 0.16 and 0.20 with say 40 increments and use the last coordinate output as the point. Which would give

| | | | | | | | | | | | | | | | | | | | | | |
|---------|--------|--------|--------|---------|--------|----------|--------|---------|--------|--------|--------|---------|----------|--------|--------|---------|---------|--------|---------|--|--|
| ----- | | | | | | | | | | | | | | | | | | | | | |
| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(cd) | h(cd) | x(g) | z(g) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) | ca(pl) | k(pl) | | |
| 5.00 | 745.7 | 0.6883 | 0.5623 | 0.06828 | 0.4541 | 0.5972 | 0.8457 | 0.03011 | 0.1862 | 0.2889 | 0.3606 | 0.01190 | 0.002875 | 0.8127 | 0.4927 | 0.1530 | 0.01126 | 0.5480 | 0.02379 | | |
| ----- | | | | | | | | | | | | | | | | | | | | | |
| mode | bi | cd | g | liq | ksp | pl | sill | q | | | | | | | | | | | | | |
| 0.195 | 0.1548 | 0.1075 | 0.1204 | 0.1568 | 0.1260 | 7.474e-5 | 0 | 0.3344 | | | | | | | | | | | | | |

here the mode of pl is so low as to be effectively zero and at the (sill pl) point.

```
% -----
i1  bi cd g liq ksp pl q  - sill
0.1950 5.00 745.7 % sill = 0
```

3) you could run the equilibria over a small P range and use the interpolation function in drawpd to set it at 5 kbar (this is what the 'x 2 5' script at the top does. This is the way I will do it below (though admittedly I do tend to use method 1 & 2 more often, though they can cause trouble). This approach produces a list of numbers rather than just one point. Doing it this way may give a result like:

```
% -----
il  bi cd g liq ksp q  - pl sill

0.1000 5.23 748.9 % pl = 0sill = 0
0.1200 5.18 748.2 % pl = 0sill = 0
0.1400 5.13 747.6 % pl = 0sill = 0
0.1600 5.09 746.9 % pl = 0sill = 0
0.1800 5.04 746.2 % pl = 0sill = 0
0.2000 4.99 745.6 % pl = 0sill = 0
0.2200 4.94 744.9 % pl = 0sill = 0
0.2400 4.89 744.3 % pl = 0sill = 0
0.2600 4.84 743.7 % pl = 0sill = 0
0.2800 4.79 743.1 % pl = 0sill = 0
0.3000 4.74 742.5 % pl = 0sill = 0
```

Just from visual inspection we can see the point must lie between 0.1800 and 0.2000, consistent with what we got for approach 2.

To calculate this list I entered the following:

```
choose from: ged anth bi cd st ctd chl g sp mu pa opx liq ksp pl osm ky sill and q H2O
which phases : =
use same phases - of these: bi cd g liq ksp pl sill q
omit :
no phases in excess (from script)

variance of required equilibria :
  0 = invariant
  1 = univariant
  2 = divariant
  ...
  n = n-variant
variance : 2
you may set zero modal proportions, from:bi cd g liq ksp pl sill q
which to set : sill pl

specification of PT window:
PT window within which invariant points expected to lie
T low,high, P low,high : 600 900 4 6
making a bulk composition range within the range specified,
start and finish proportions across bulk composition range : 0.1 0.3
how many increments (max = 100) : 10
```

The key info is highlighted, especially important is manually entering a T & P range (with the P range limits being either side of the P of the T-x pseudosection (ie 5kbar)). The start and finish proportions must also straddle the likely x value for the point.

Putting the three lines and the point into your drawpd file, and setting the start / finish points where needed ie the following headers:

```
% -----
i1  bi cd g liq ksp q - pl sill
```

```
% -----
u1  bi liq ksp pl sill q - g
```

```
begin end
```

```
% -----
u2  bi g liq ksp pl sill q - cd
```

```
begin end
```

```
% -----
u3  bi cd g liq ksp pl q - sill
```

```
begin i1
```

and running drawpd should give (line numbers blue, variance in circles):

+q +ksp +liq



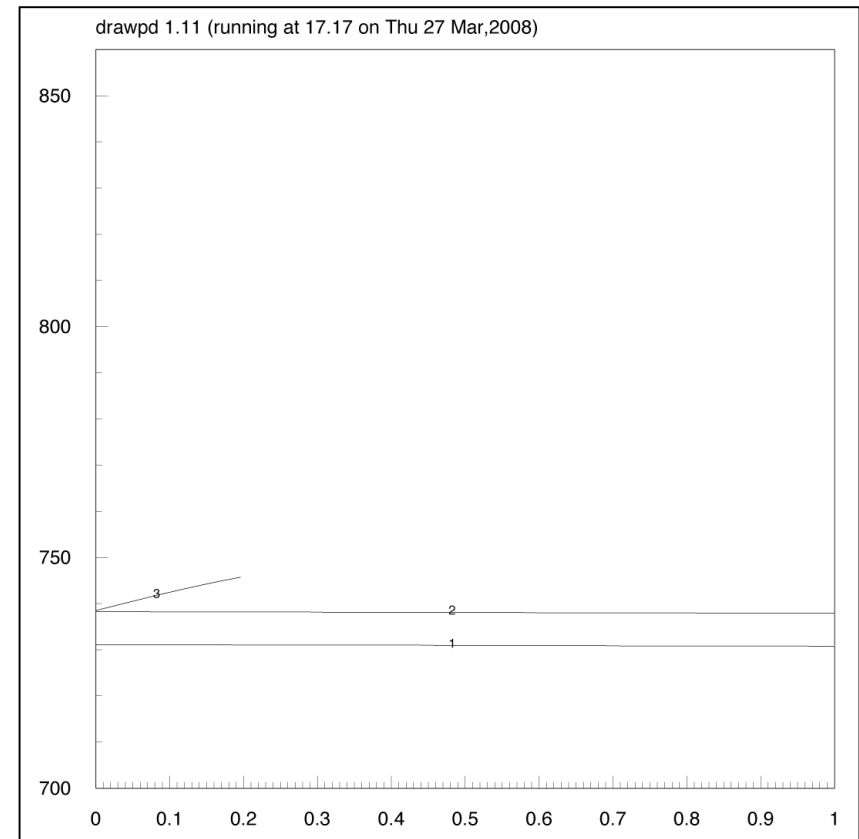
The next line to calculate is the (pl) line that emanates from the (sill pl) point and bounds the g-cd-sill-bi-ksp-pl-q-liq divariant field. It runs from i1 to the right hand side of the diagram so in drawpd it should have the header:

```
% -----
u4  bi cd g liq ksp sill q - pl
```

```
i1 end
```

From i1 there will be two more lines to calculate from the two trivariant fields. These will be (pl) from the g-cd-bi-ksp-pl-q-liq field and (sill) from the g-cd-sill-bi-ksp-q-liq field calculating these gives

```
% -----
```



```

u5   bi cd g liq ksp q  - pl

begin i1

0.0300 5.00 754.3 % pl = 0
0.0600 5.00 752.7 % pl = 0
0.0900 5.00 751.2 % pl = 0
0.1200 5.00 749.7 % pl = 0
0.1500 5.00 748.1 % pl = 0
0.1800 5.00 746.5 % pl = 0
0.2100 5.00 745.0 % pl = 0
0.2400 5.00 743.4 % pl = 0
0.2700 5.00 741.9 % pl = 0
0.3000 5.00 740.3 % pl = 0

% -----
u6   bi cd g liq ksp q  - sill

i1 end

0 5.00 733.5 % sill = 0
0.0400 5.00 736.2 % sill = 0
0.0800 5.00 738.9 % sill = 0
0.1200 5.00 741.4 % sill = 0
0.1600 5.00 743.7 % sill = 0
0.2000 5.00 745.9 % sill = 0
0.2400 5.00 747.9 % sill = 0
0.2800 5.00 749.8 % sill = 0
0.3200 5.00 751.5 % sill = 0
0.3600 5.00 753.0 % sill = 0
0.4000 5.00 754.5 % sill = 0

```

Looking at the output, you will notice that the (pl) line runs out of cd to low x and the (sill) line runs out of bi to higher x. This means there are two more points to calculate. These will be (pl cd) from the g-cd-bi-kspl-q-liq field and (sill bi) from the g-cd-sill-bi-kspl-q-liq field. Calculating first the (pl cd) point from the g-cd-bi-kspl-q-liq field. I used the following ranges

```

you may set zero modal proportions, from:bi cd g liq ksp pl q
which to set : pl cd

```

```

specification of PT window:
PT window within which invariant points expected to lie
T low,high, P low,high : 600 900 4.5 5.5
making a bulk composition range within the range specified,
start and finish proportions across bulk composition range : 0 0.05
how many increments (max = 100) : 10

```

and got the result

```

% -----
i2   bi g liq ksp q  - cd pl

```

```

0 4.69 758.1 % cd = 0pl = 0
0.0050 4.83 756.8 % cd = 0pl = 0
0.0100 4.97 755.5 % cd = 0pl = 0
0.0150 5.12 754.1 % cd = 0pl = 0
0.0200 5.27 752.7 % cd = 0pl = 0
0.0250 5.43 751.3 % cd = 0pl = 0

```

which means the point will lie very close to the left hand edge between $x=0.0100$ and $x=0.0150$.

for the (sill bi) point from the g-cd-sill-bi-ksp-q-liq field I used the ranges:

```

specification of PT window:
PT window within which invariant points expected to lie
T low,high, P low,high : 600 900 4.5 5.5
making a bulk composition range within the range specified,
start and finish proportions across bulk composition range : 0.3 0.5
how many increments (max = 100) : 10

```

and got the result

```

% -----
i3  cd g liq ksp q - bi sill

0.3200 5.45 764.1 % bi = 0sill = 0
0.3400 5.34 761.5 % bi = 0sill = 0
0.3600 5.22 759.1 % bi = 0sill = 0
0.3800 5.11 756.8 % bi = 0sill = 0
0.4000 5.00 754.6 % bi = 0sill = 0
0.4200 4.90 752.5 % bi = 0sill = 0
0.4400 4.79 750.4 % bi = 0sill = 0
0.4600 4.69 748.5 % bi = 0sill = 0
0.4800 4.60 746.7 % bi = 0sill = 0
0.5000 4.51 745.0 % bi = 0sill = 0

```

so the headers for u5 and u6 should now read

```

% -----
u5  bi cd g liq ksp q - pl

i2  i1

```

and

```

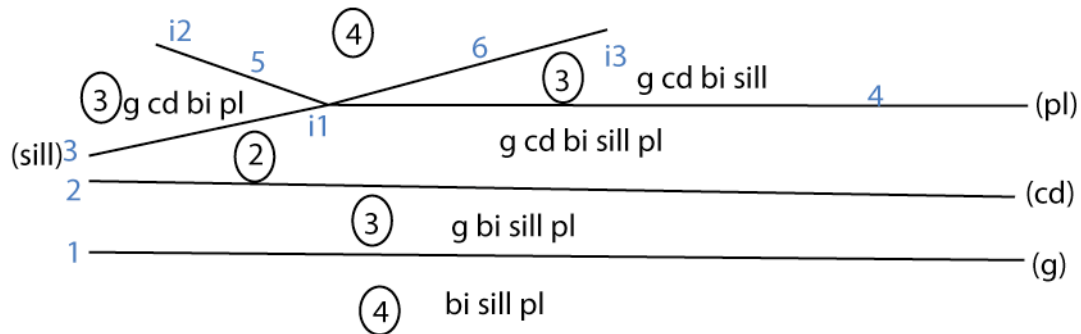
% -----
u6  bi cd g liq ksp q - sill

i1 i3

```

and your sketch like (notice I have not tried to draw the sketch to scale, that's what drawpd is for)

+q +ksp +liq



Now, the other lines around i2 may be a bit tricky to calculate as they only cover a very short segment of the x range. Starting with the (cd) line bounding the g-cd-bi-ksp-pl-q-liq field, I used the following x ranges and increments

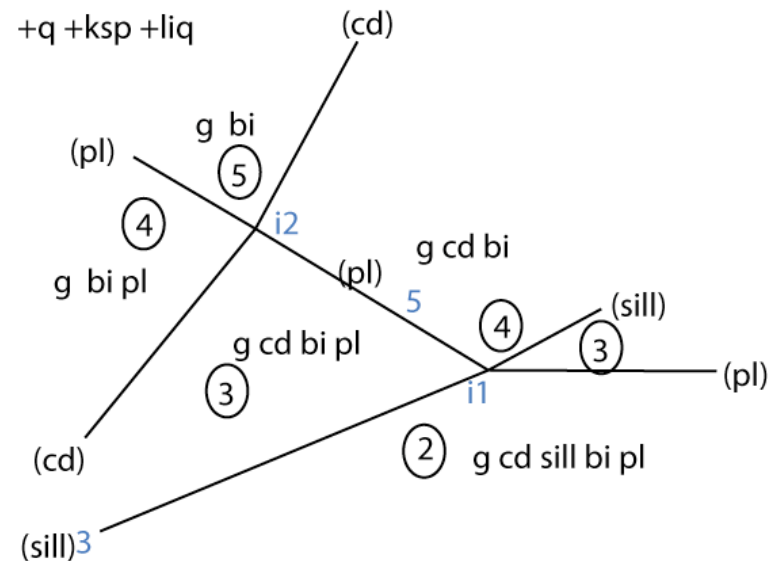
start and finish proportions across bulk composition range : 0 0.02
how many increments (max = 100) : 10

and got the result-with start/finish points entered:

```
% -----
u7   bi g liq ksp pl q  - cd
begin i2
0 5.00 744.4 % cd = 0
0.0020 5.00 746.5 % cd = 0
0.0040 5.00 748.5 % cd = 0
0.0060 5.00 750.5 % cd = 0
0.0080 5.00 752.5 % cd = 0
0.0100 5.00 754.4 % cd = 0
```

and a sketch of what the phase relationships around this point should look like is to the right

calculating the (pl) line bounding the g-bi-pl-ksp-q-liq field which must go from the left hand edge to i2 using the following ranges



making a bulk composition range within the range specified,
start and finish proportions across bulk composition range : 0 0.02
how many increments (max = 100) : 5

gives the result

```
% -----  
u8    bi g liq ksp q  - pl  
  
begin  i2  
  
0 5.00 756.3  % pl = 0  
0.0040 5.00 755.9  % pl = 0  
0.0080 5.00 755.5  % pl = 0  
0.0120 5.00 755.1  % pl = 0  
0.0160 5.00 754.7  % pl = 0  
0.0200 5.00 754.4  % pl = 0
```

The slope and extent of the (cd) line bounding the g-cd-bi-ksp-q-liq field is still unknown, so I calculated from x=0 to x=0.5 (15 increments) just to see where it goes and got the result:

```
% -----  
u<k>    bi g liq ksp q  - cd  
  
begin  end  
  
0 5.00 736.3  % cd = 0  
0.0333 5.00 774.9  % cd = 0  
0.0667 5.00 795.1  % cd = 0
```

This means it is fairly steep, so I recalculate it over a smaller range to get a few more points ie:

making a bulk composition range within the range specified,
start and finish proportions across bulk composition range : 0 0.1
how many increments (max = 100) : 10

getting the result

```
% -----  
u9    bi g liq ksp q  - cd  
  
i2  end  
  
0 5.00 736.3  % cd = 0  
0.0100 5.00 754.1  % cd = 0  
0.0200 5.00 764.5  % cd = 0  
0.0300 5.00 772.5  % cd = 0
```

```

0.0400 5.00 779.4 % cd = 0
0.0500 5.00 785.7 % cd = 0
0.0600 5.00 791.4 % cd = 0
0.0700 5.00 796.9 % cd = 0
0.0800 5.00 802.1 % cd = 0
0.0900 5.00 807.1 % cd = 0

```

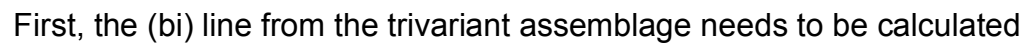
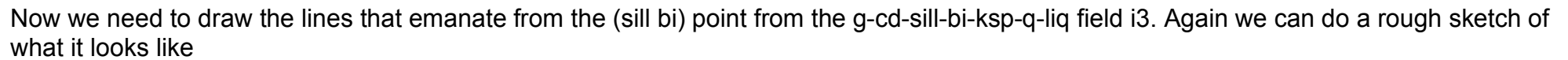
Notice , how this line terminates at a (cd bi) as bi mode goes to zero as x increases.

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

```
phases : bi, cd, g, liq, ksp, q
```

| | | | | | | | | | | | | | | | | | |
|---------|---------|--------|---------|---------|---------|--------|--------|---------|--------|--------|--------|----------|----------|--------|--------|---------|----------|
| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(cd) | h(cd) | x(g) | z(g) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) |
| 5.00 | 736.3 | 0.6606 | 0.5501 | 0.07752 | 0.4270 | 0.6009 | 0.8369 | 0.04184 | 0.1716 | 0.2946 | 0.4631 | 0.01400 | 0.002581 | 0.7994 | 0.5018 | 0.2480 | 0.02421 |
| mode | bi | cd | g | liq | ksp | q | | | | | | | | | | | |
| 0 | 0.2757 | 0 | 0.08565 | 0.1155 | 0.08495 | 0.4383 | | | | | | | | | | | |
| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(cd) | h(cd) | x(g) | z(g) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) |
| 5.00 | 754.1 | 0.6295 | 0.5134 | 0.09123 | 0.4101 | 0.5820 | 0.8164 | 0.02939 | 0.1870 | 0.2999 | 0.3841 | 0.01200 | 0.003822 | 0.7910 | 0.4817 | 0.1747 | 0.01247 |
| mode | bi | cd | g | liq | ksp | q | | | | | | | | | | | |
| 0.010 | 0.2153 | 0 | 0.1290 | 0.1664 | 0.09314 | 0.3961 | | | | | | | | | | | |
| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(cd) | h(cd) | x(g) | z(g) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) |
| 5.00 | 802.1 | 0.4975 | 0.3904 | 0.1429 | 0.3327 | 0.5187 | 0.7292 | 0.01310 | 0.2257 | 0.3216 | 0.2181 | 0.008431 | 0.01001 | 0.7455 | 0.4200 | 0.09147 | 0.004895 |
| mode | bi | cd | g | liq | ksp | q | | | | | | | | | | | |
| 0.080 | 0.03096 | 0 | 0.2587 | 0.3625 | 0.09785 | 0.2500 | | | | | | | | | | | |
| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(cd) | h(cd) | x(g) | z(g) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) |
| 5.00 | 807.1 | 0.4810 | 0.3768 | 0.1480 | 0.3230 | 0.5105 | 0.7171 | 0.01223 | 0.2292 | 0.3247 | 0.2069 | 0.008225 | 0.01096 | 0.7389 | 0.4128 | 0.08721 | 0.004622 |
| mode | bi | cd | g | liq | ksp | q | | | | | | | | | | | |
| 0.090 | 0.01228 | 0 | 0.2713 | 0.3878 | 0.09533 | 0.2334 | | | | | | | | | | | |

we will return to that point later, but for now, these lines need to go in your dr d file. Running draw pd, the results should look like:



```
% -----
u10   cd g liq ksp sill q - bi

i3 end

0.4400 5.00 754.5 % bi = 0
0.4800 5.00 754.5 % bi = 0
0.5200 5.00 754.4 % bi = 0
0.5600 5.00 754.4 % bi = 0
0.6000 5.00 754.4 % bi = 0
0.6400 5.00 754.4 % bi = 0
0.6800 5.00 754.3 % bi = 0
0.7200 5.00 754.3 % bi = 0
0.7600 5.00 754.3 % bi = 0
0.8000 5.00 754.3 % bi = 0
0.8400 5.00 754.3 % bi = 0
0.8800 5.00 754.2 % bi = 0
0.9200 5.00 754.2 % bi = 0
0.9600 5.00 754.2 % bi = 0
1.0000 5.00 754.2 % bi = 0
```

Then the (sill) line from the g-cd-sill-ksp-q-liq quadrivariant field and the (bi) line from the g-cd-bi-ksp-q-liq field need to be calculated. Note that this second line should terminate at the (cd bi) point at the end of u9 that we know is there but have not calculated yet. The two new lines are

```
% -----
u11   cd g liq ksp q - sill

i3 end

0.3000 5.00 614.2 % sill = 0
0.3280 5.00 654.1 % sill = 0
0.3560 5.00 692.9 % sill = 0
0.3840 5.00 731.7 % sill = 0
0.4120 5.00 769.7 % sill = 0
0.4400 5.00 806.1 % sill = 0
0.4680 5.00 838.5 % sill = 0
0.4960 5.00 864.8 % sill = 0
0.5240 5.00 885.0 % sill = 0

% -----
u12   cd g liq ksp q - bi

begin i3

0.1000 5.00 809.9 % bi = 0
0.1200 5.00 806.5 % bi = 0
0.1400 5.00 803.0 % bi = 0
0.1600 5.00 799.4 % bi = 0
0.1800 5.00 795.8 % bi = 0
0.2000 5.00 792.0 % bi = 0
0.2200 5.00 788.2 % bi = 0
0.2400 5.00 784.4 % bi = 0
```



```

0.2600 5.00 780.5 % bi = 0
0.2800 5.00 776.7 % bi = 0
0.3000 5.00 772.8 % bi = 0
0.3200 5.00 769.0 % bi = 0
0.3400 5.00 765.3 % bi = 0
0.3600 5.00 761.6 % bi = 0
0.3800 5.00 758.1 % bi = 0
0.4000 5.00 754.6 % bi = 0
0.4200 5.00 751.3 % bi = 0
0.4400 5.00 748.1 % bi = 0
0.4600 5.00 745.1 % bi = 0
0.4800 5.00 742.2 % bi = 0
0.5000 5.00 739.5 % bi = 0

```

There are a couple of things to note about these lines. The first line, u11, is fairly steep, and although it terminates at a (sill q) point, this is out of our T-x window of interest. However that does not mean the (q) lines that emanate from this point do not track back into our T-x window. From the on-screen output the second line (u12) does indeed terminate at a (cd bi) point at low x and $T \approx 810^\circ\text{C}$.

We could then go and calculate the (cd bi) point where u9 and u12 intersect, and admittedly this is what I initially did. However, at these T conditions and at low xAl₂O₃ we should consider opx becoming stable. Again it is useful to consider this in terms of what happens in an AFM diagram in KFMASH.

Now that we think an (opx) line could occur, we need to consider what field it may bound. As opx-sill will not be stable at these pressures, we need only consider the sillimanite absent assemblages. Furthermore the opx is most likely to be present on the low x side of the diagram. Often looking for a new phase in the higher variance assemblages is easier as the lines may extend across the lower variance fields and are thus harder to miss.

So looking for an opx in line bounding the g-bi field is where I will start as this is the lowest xAl₂O₃. The (opx) line from the assemblage g-bi-opx-q-ksp-liq (v=4) does return values in the right T range so we have opx appearing.

```

which phases : bi g opx ksp q liq
no phases in excess (from script)

```

```

variance of required equilibria :

```

```

    0 = invariant

```

```

    1 = univariant

```

```

    2 = divariant

```

```

    ...

```

```

    n = n-variant

```

```

variance : 4

```

```

you may set zero modal proportions, from:bi g opx liq ksp q

```

```

which to set : opx

```

```

specification of PT window:

```

```

P range over which T of reactions to be calculated

```

```

P window: P low,high :

```

```

T window within which reactions expected to lie

```

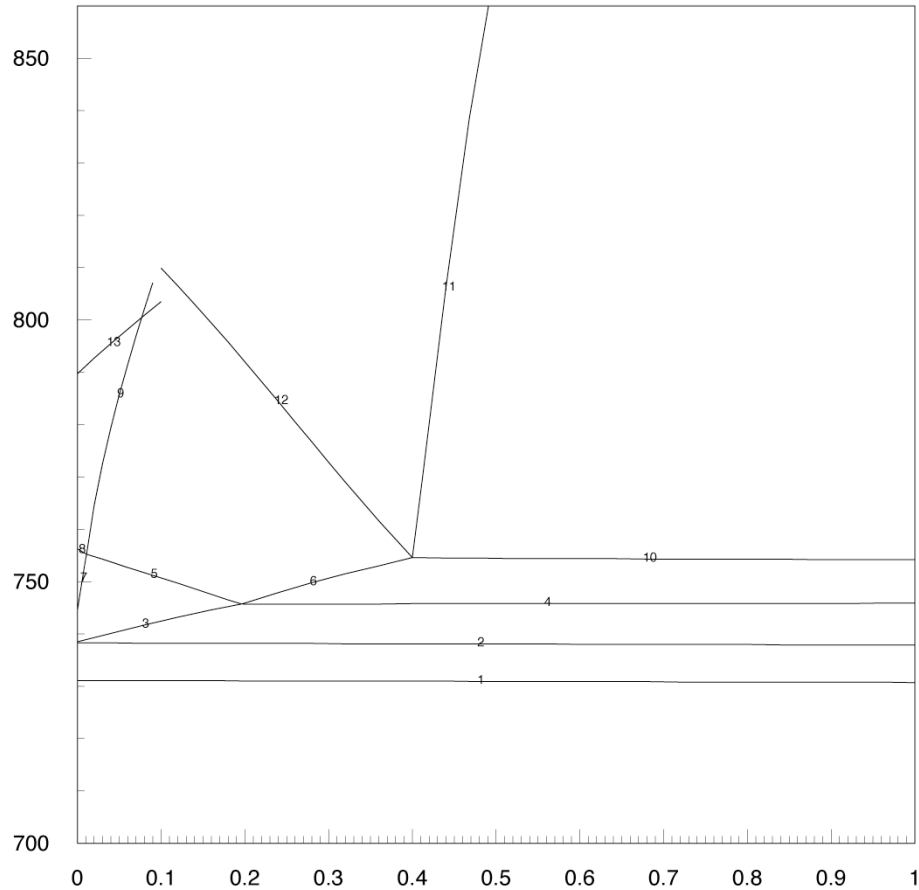
T window: T low,high :
 making a bulk composition range within the range specified,
 start and finish proportions across bulk composition range : 0 0.2
 how many increments (max = 100) : 10

| | | | | | | | | | | | | | | | | | | |
|---------|----------|--------|--------|--------|---------|---------|--------|--------|--------|--------|--------|--------|----------|----------|--------|--------|---------|----------|
| ----- | | | | | | | | | | | | | | | | | | |
| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(g) | z(g) | x(opx) | y(opx) | Q(opx) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) |
| 5.00 | 789.7 | 0.5767 | 0.3678 | 0.1364 | 0.7862 | 0.02102 | 0.6265 | 0.1325 | 0.3858 | 0.2130 | 0.3190 | 0.2820 | 0.009341 | 0.01119 | 0.7826 | 0.4378 | 0.1214 | 0.006508 |
| mode | bi | g | opx | liq | ksp | q | | | | | | | | | | | | |
| 0 | 0.1326 | 0.1815 | 0 | 0.2648 | 0.09159 | 0.3294 | | | | | | | | | | | | |
| ----- | | | | | | | | | | | | | | | | | | |
| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(g) | z(g) | x(opx) | y(opx) | Q(opx) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) |
| 5.00 | 792.7 | 0.5583 | 0.3749 | 0.1380 | 0.7734 | 0.01855 | 0.6128 | 0.1371 | 0.3911 | 0.2163 | 0.3193 | 0.2641 | 0.009060 | 0.01085 | 0.7741 | 0.4338 | 0.1124 | 0.005981 |
| mode | bi | g | opx | liq | ksp | q | | | | | | | | | | | | |
| 0.020 | 0.1076 | 0.2007 | 0 | 0.2874 | 0.09380 | 0.3105 | | | | | | | | | | | | |
| ----- | | | | | | | | | | | | | | | | | | |
| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(g) | z(g) | x(opx) | y(opx) | Q(opx) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) |
| 5.00 | 795.5 | 0.5391 | 0.3819 | 0.1394 | 0.7598 | 0.01647 | 0.5986 | 0.1417 | 0.3955 | 0.2194 | 0.3196 | 0.2478 | 0.008828 | 0.01047 | 0.7651 | 0.4298 | 0.1047 | 0.005563 |
| mode | bi | g | opx | liq | ksp | q | | | | | | | | | | | | |
| 0.040 | 0.08255 | 0.2198 | 0 | 0.3106 | 0.09574 | 0.2913 | | | | | | | | | | | | |
| ----- | | | | | | | | | | | | | | | | | | |
| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(g) | z(g) | x(opx) | y(opx) | Q(opx) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) |
| 5.00 | 798.2 | 0.5195 | 0.3889 | 0.1405 | 0.7455 | 0.01470 | 0.5839 | 0.1463 | 0.3989 | 0.2223 | 0.3201 | 0.2332 | 0.008637 | 0.01007 | 0.7557 | 0.4257 | 0.09794 | 0.005227 |
| mode | bi | g | opx | liq | ksp | q | | | | | | | | | | | | |
| 0.060 | 0.05773 | 0.2388 | 0 | 0.3343 | 0.09738 | 0.2718 | | | | | | | | | | | | |
| ----- | | | | | | | | | | | | | | | | | | |
| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(g) | z(g) | x(opx) | y(opx) | Q(opx) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) |
| 5.00 | 800.9 | 0.4996 | 0.3959 | 0.1412 | 0.7306 | 0.01318 | 0.5691 | 0.1510 | 0.4010 | 0.2250 | 0.3207 | 0.2199 | 0.008479 | 0.009656 | 0.7460 | 0.4216 | 0.09206 | 0.004952 |
| mode | bi | g | opx | liq | ksp | q | | | | | | | | | | | | |
| 0.080 | 0.03320 | 0.2575 | 0 | 0.3584 | 0.09870 | 0.2522 | | | | | | | | | | | | |
| ----- | | | | | | | | | | | | | | | | | | |
| P(kbar) | T(?C) | x(bi) | y(bi) | Q(bi) | x(g) | z(g) | x(opx) | y(opx) | Q(opx) | q(L) | fsp(L) | na(L) | an(L) | ol(L) | x(L) | h2o(L) | na(ksp) | ca(ksp) |
| 5.00 | 803.5 | 0.4798 | 0.4028 | 0.1415 | 0.7152 | 0.01186 | 0.5541 | 0.1556 | 0.4019 | 0.2274 | 0.3214 | 0.2080 | 0.008345 | 0.009231 | 0.7359 | 0.4175 | 0.08689 | 0.004723 |
| mode | bi | g | opx | liq | ksp | q | | | | | | | | | | | | |
| 0.100 | 0.009060 | 0.2759 | 0 | 0.3828 | 0.09969 | 0.2326 | | | | | | | | | | | | |

this will be line u13

Putting this line in the draw file and running drawpd we get a diagram that looks like:

drawpd 1.11 (running at 17.10 on Sun 23 Nov,2008)



So our new line crosses into the existing g-bi-cd-ksp-q-liq field and we will have to calculate this lower variance line and also the point where lines 9 & 13 cross (cd opx). Looking at the diagram above, we can see that the (opx) line for the assemblage g-bi-cd-opx-ksp-q-liq is likely to be short so we should use plenty of increments to calculate it. eg

which phases : bi g opx liq ksp q cd
no phases in excess (from script)

variance of required equilibria :

0 = invariant
1 = univariant
2 = divariant
...
n = n-variant

variance : 3
 you may set zero modal proportions, from:bi cd g opx liq ksp q
 which to set : opx

specification of PT window:
 P range over which T of reactions to be calculated
 P window: P low,high :
 T window within which reactions expected to lie
 T window: T low,high :
 making a bulk composition range within the range specified,
 start and finish proportions across bulk composition range : 0 0.2
 how many increments (max = 100) : 20

When you calculate this you can see that the line starts at a (opx cd) point and ends at a (opx bi) point, with the dr output being

```
% -----
u14  bi cd g liq ksp q  - opx

begin  end

0.0800 5.00 800.5 % opx = 0
0.0900 5.00 800.7 % opx = 0
0.1000 5.00 800.8 % opx = 0
0.1100 5.00 800.9 % opx = 0
0.1200 5.00 801.1 % opx = 0
0.1300 5.00 801.2 % opx = 0
0.1400 5.00 801.3 % opx = 0
```

calculating these two terminating points gives

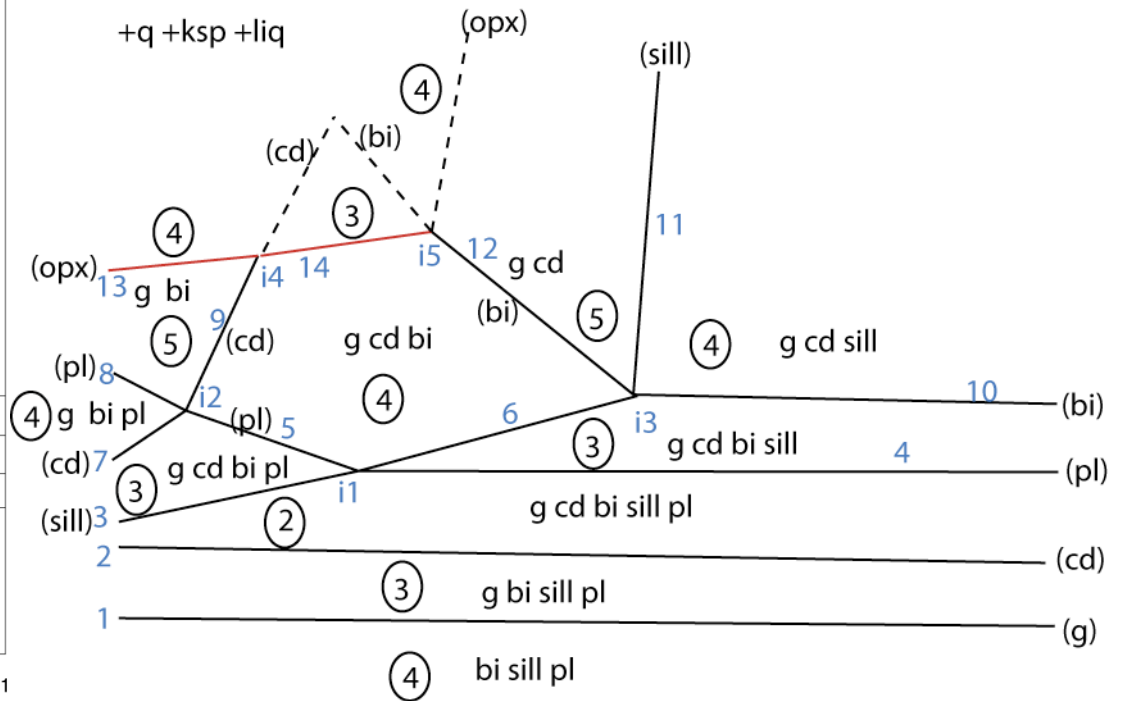
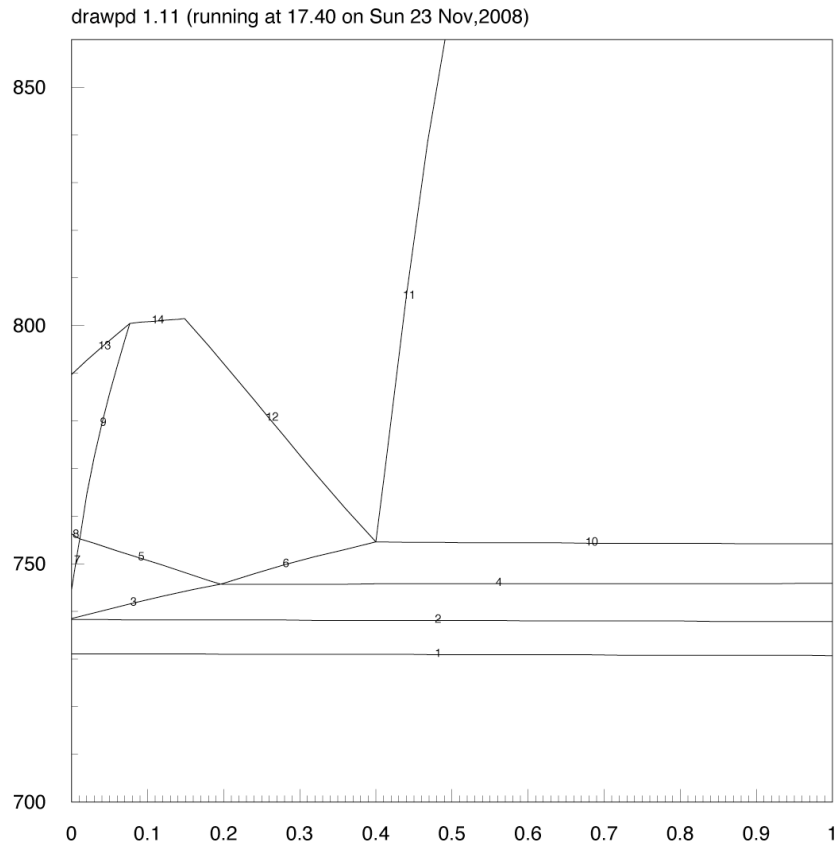
```
% -----
i4  bi g liq ksp q  - cd opx

0.0650 4.85 797.4 % cd = 0opx = 0
0.0700 4.91 798.7 % cd = 0opx = 0
0.0750 4.98 800.0 % cd = 0opx = 0
0.0800 5.04 801.3 % cd = 0opx = 0
0.0850 5.10 802.6 % cd = 0opx = 0
0.0900 5.16 803.9 % cd = 0opx = 0

% -----
i5  cd g liq ksp q  - bi opx

0.1200 5.19 804.8 % bi = 0opx = 0
0.1300 5.13 803.7 % bi = 0opx = 0
0.1400 5.06 802.5 % bi = 0opx = 0
0.1500 4.99 801.3 % bi = 0opx = 0
0.1600 4.92 800.1 % bi = 0opx = 0
0.1700 4.85 798.9 % bi = 0opx = 0
```

which also terminate lines u9 (i4) and u12 (i5). Putting this together in draw pd gives



The two other lines around i4 and i5 need to be calculated (see the dashed lines in the sketch above)

Starting with the (bi) and (cd) lines. The (bi) line below is very flat so the (cd) line may be very short.

```
% -----
u15   cd g opx liq ksp q   - bi

begin end

0.0600 5.00 801.7 % bi = 0
0.0700 5.00 801.6 % bi = 0
0.0800 5.00 801.6 % bi = 0
0.0900 5.00 801.6 % bi = 0
```

```

0.1000 5.00 801.6 % bi = 0
0.1100 5.00 801.5 % bi = 0
0.1200 5.00 801.5 % bi = 0
0.1300 5.00 801.5 % bi = 0
0.1400 5.00 801.5 % bi = 0

```

Even with small increments I could not calculate the (cd) line, so I decided to change the starting guesses, using the following from the (bi) calculation

```

% calculated at P = 5.0; T = 801
readxyz x(bi)      0.5045
readxyz y(bi)      0.3955
readxyz Q(bi)      0.1406
readxyz x(cd)      0.3373
readxyz h(cd)      0.5211
readxyz x(g)       0.7335
readxyz z(g)       0.01283
readxyz x(opx)     0.5727
readxyz y(opx)     0.1508
readxyz Q(opx)     0.3999
readxyz q(L)       0.2265
readxyz fsp(L)     0.3199
readxyz na(L)      0.2085
readxyz an(L)      0.008249
readxyz ol(L)      0.009817
readxyz x(L)       0.7484
readxyz h2o(L)     0.4211
readxyz na(ksp)    0.08639
readxyz ca(ksp)    0.004676

```

You can find this set of numbers at the bottom of the THERMOCALC script file for this tutorial. Using the new starting guesses fixed the problem and I got:

```

% -----
u16  bi g opx liq ksp q - cd

begin end

0.0600 5.00 801.5 % cd = 0
0.0650 5.00 801.2 % cd = 0
0.0700 5.00 800.9 % cd = 0
0.0750 5.00 800.6 % cd = 0

```

These last two lines intersect at a point (bi cd)

```

% -----
i6  g opx liq ksp q - bi cd

```

```

0.0400 4.89 799.9 % bi = 0cd = 0
0.0600 5.03 802.2 % bi = 0cd = 0
0.0800 5.17 804.4 % bi = 0cd = 0

```

We now have to calculate the remaining lines that emanate from i5 & i6. Starting with the remaining (opx) line from i5, you will discover that this line is rather steep and will require closely spaced increments. Using the range and increments below

```

start and finish proportions across bulk composition range : 0.1 0.3
how many increments (max = 100) : 40

```

I got the result

```

% -----
u17   cd g liq ksp q  - opx

i5   end

0.1500 5.00 810.8 % opx = 0
0.1550 5.00 833.0 % opx = 0
0.1600 5.00 847.0 % opx = 0
0.1650 5.00 857.5 % opx = 0
0.1700 5.00 866.0 % opx = 0

```

The two remaining lines from i6 (bi) & (cd) can now be calculated. Again, you will find that the (cd) line is steep. Below are the draw pd data for these.

```

% -----
u18   g opx liq ksp q  - cd

i6   end

0.0450 5.00 762.6 % cd = 0
0.0500 5.00 781.0 % cd = 0
0.0550 5.00 798.8 % cd = 0
0.0600 5.00 816.2 % cd = 0
0.0650 5.00 833.2 % cd = 0
0.0700 5.00 850.1 % cd = 0
0.0750 5.00 867.1 % cd = 0

```

```

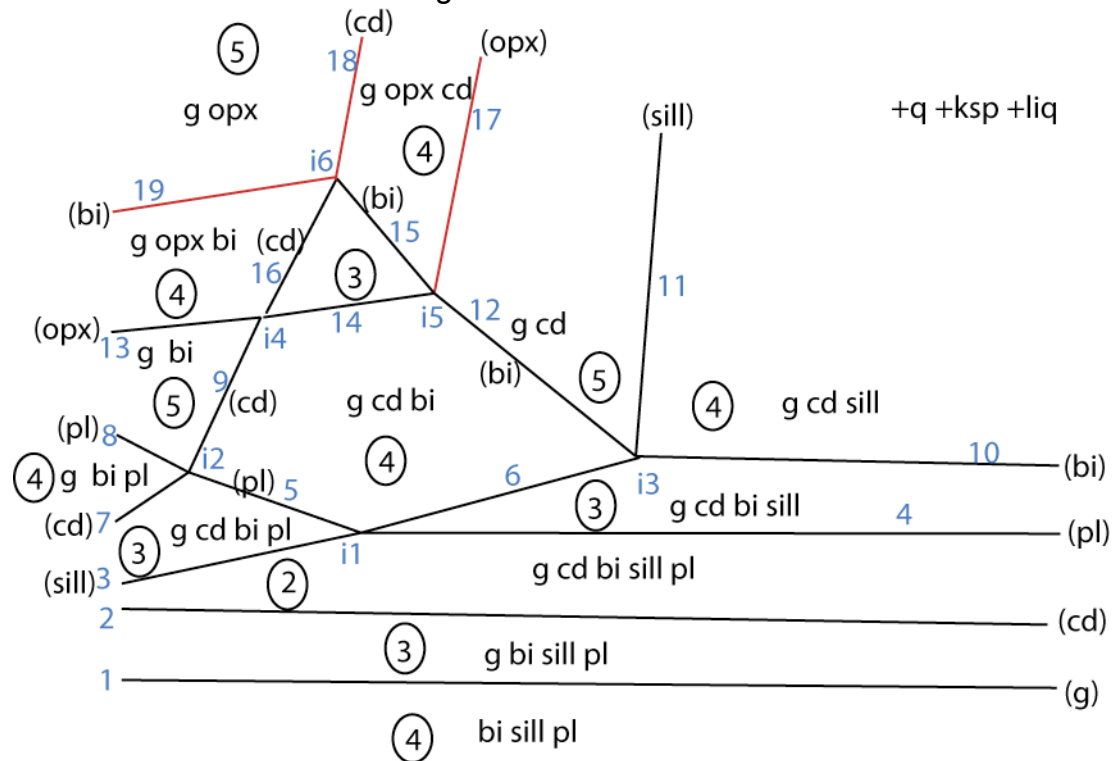
% -----
u19   g opx liq ksp q  - bi

begin i6

```

```
0 5.00 798.7 % bi = 0
0.0100 5.00 799.3 % bi = 0
0.0200 5.00 799.8 % bi = 0
0.0300 5.00 800.3 % bi = 0
0.0400 5.00 800.8 % bi = 0
0.0500 5.00 801.4 % bi = 0
0.0600 5.00 801.9 % bi = 0
0.0700 5.00 802.4 % bi = 0
0.0800 5.00 803.0 % bi = 0
0.0900 5.00 803.5 % bi = 0
0.1000 5.00 804.0 % bi = 0
```

below is the sketch for the diagram thus far



If you look at the output for lines u17 and u19 you will see that they terminate at (opx ksp) and (cd ksp) points respectively, but that these points are outside our window of interest. However, this does not preclude any of the (ksp) lines from these points re-entering our PT window.

Before we look at the possible (ksp) equilibria, we need to consider if any other new phases come in. In particular hercynitic spinel may occur to higher $x\text{Al}_2\text{O}_3$ if the $x\text{Fe}$ of this rock is high enough.

Following similar logic to that used for opx, we would expect spinel to occur at high $x\text{Al}_2\text{O}_3$ and high T. The (sp) line in the assemblage g-cd-sill-q-ksp-liq can be calculated

```
% -----  
u<k>   cd g liq ksp sill q  - sp  
  
begin  end  
  
0.5200 5.00 866.8 % sp = 0  
0.5600 5.00 866.8 % sp = 0  
0.6000 5.00 866.8 % sp = 0  
0.6400 5.00 866.8 % sp = 0  
0.6800 5.00 866.9 % sp = 0  
0.7200 5.00 866.9 % sp = 0  
0.7600 5.00 866.9 % sp = 0  
0.8000 5.00 867.0 % sp = 0  
0.8400 5.00 867.0 % sp = 0  
0.8800 5.00 867.0 % sp = 0  
0.9200 5.00 867.1 % sp = 0  
0.9600 5.00 867.1 % sp = 0  
1.0000 5.00 867.1 % sp = 0
```

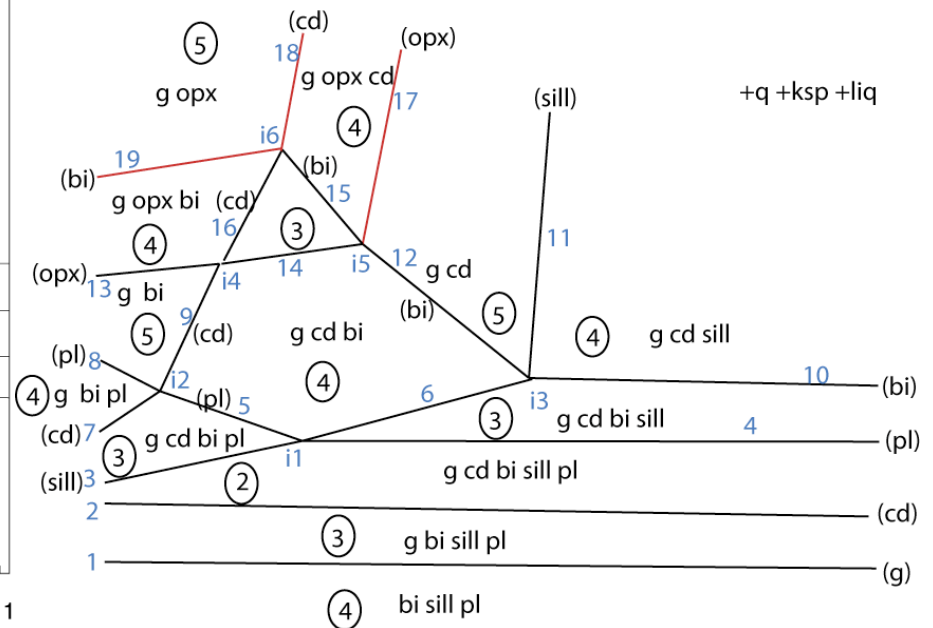
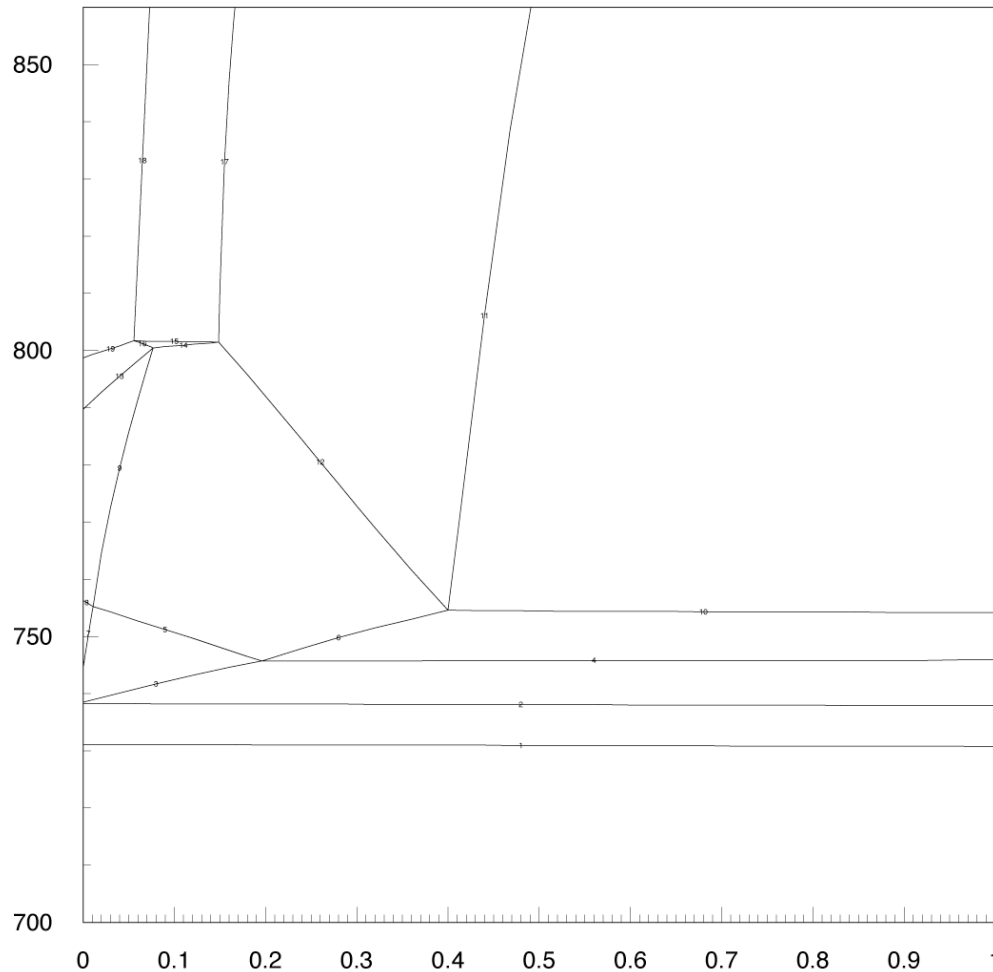
and is just outside our T-X window of interest which stops at 860°C. If you are keen, you can extend the T window to higher T and calculate the spinel-bearing equilibria but I will not cover this here.

Finally, it is worth checking what the (ksp) line discussed above does. A (ksp) line could cut across the g-opx-q-ksp-liq and/or the cd-opx-q-ksp-liq fields. Checking this shows that the (ksp) lines for these fields occur outside our window of interest:

So now all the lines and points are calculated.

The finished diagram (areas not filled) and sketch are shown below

drawpd 1.11 (running at 13.56 on Sun 28 Dec,2008)



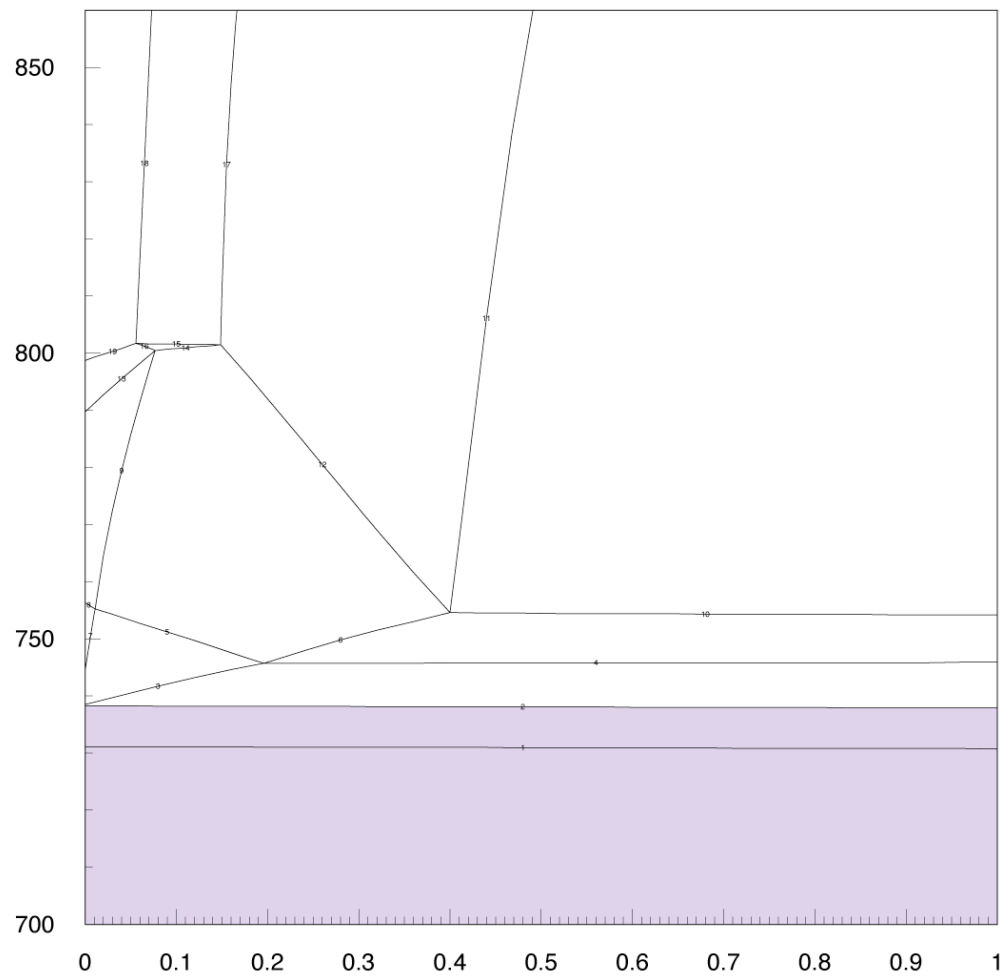
Filling in areas in T-x pseudosections.

Mostly filling in areas on T-x pseudosections is straight forward, just like in P-T pseudosections. However, things can get a bit tricky where a given line simply crosses from one side of the diagram to the other. Such as lines u1 and u2. In this case we can define the area using just one line and the area between that line and the nearest edge of the diagram will be filled. For example for u2 the code in the areas section of the drd file is

```
0.8 u2
```

and this fill the area below u2 like this:

drawpd 1.11 (running at 14.46 on Sun 28 Dec,2008)



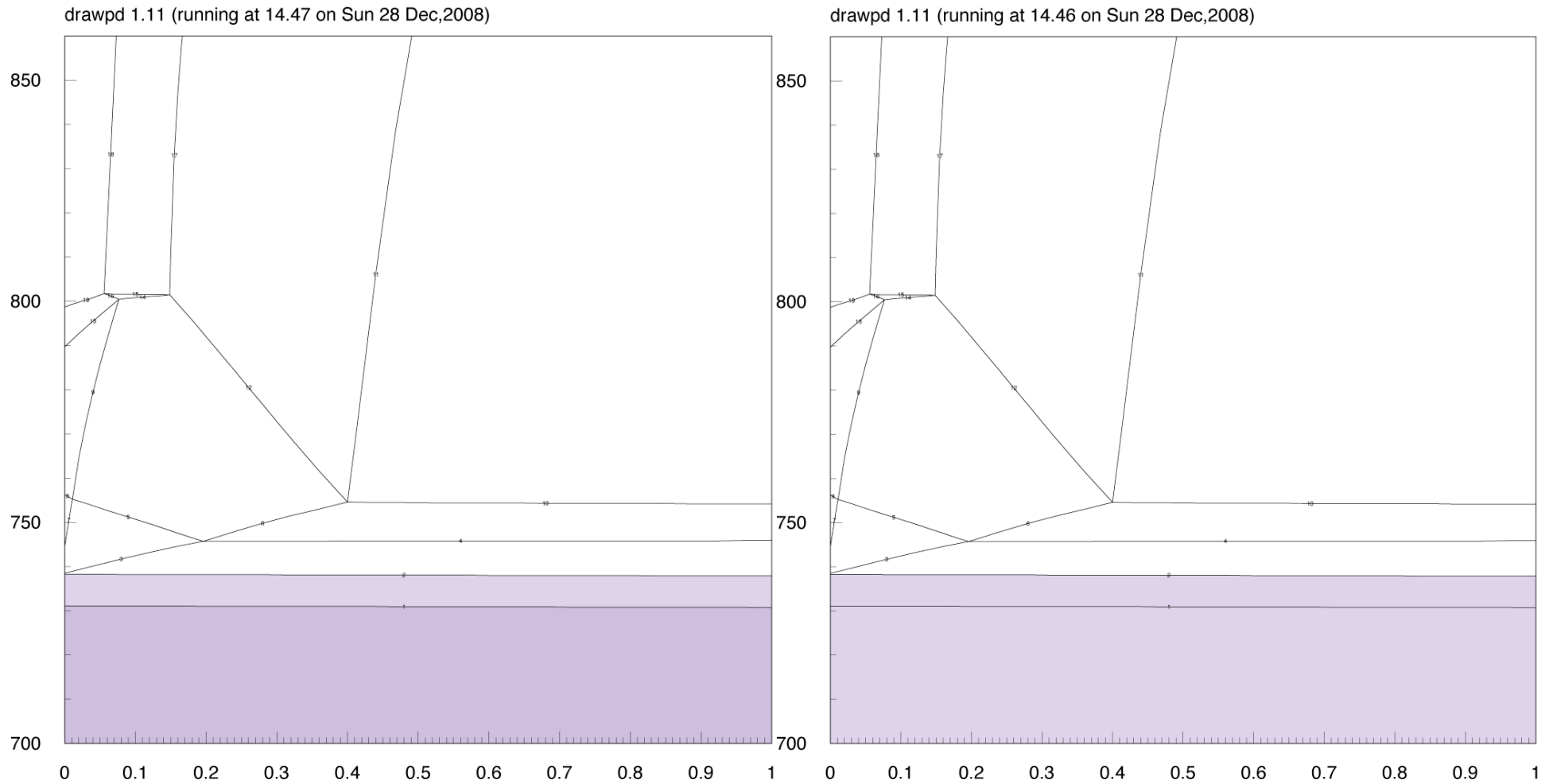
hence it is important what order you put the areas, ie

0.8 u2
0.7 u1

gives a different result than

```
0.7 u1
0.8 u2
```

as shown in the left and right hand diagrams below



Where the fill for u1 in the right hand diagram is under the fill for u2

Below is a summary of all the points and lines

- i1) bi cd g liq ksp q (pl sill)
- i2) bi g liq ksp q (cd pl)
- i3) cd g liq ksp q (bi sill)

i4) bi g liq ksp q (cd opx)
i5) cd g liq ksp q (bi opx)
i6) g opx liq ksp q (bi cd)
u1) bi liq ksp pl sill q (g) - 26 data points
u2) bi g liq ksp pl sill q (cd) - 26 data points
u3) bi cd g liq ksp pl q (sill) - 5 data points
u4) bi cd g liq ksp sill q (pl) - 21 data points
u5) bi cd g liq ksp q (pl) - 10 data points
u6) bi cd g liq ksp q (sill) - 11 data points
u7) bi g liq ksp pl q (cd) - 6 data points
u8) bi g liq ksp q (pl) - 6 data points
u9) bi g liq ksp q (cd) - 10 data points
u10) cd g liq ksp sill q (bi) - 15 data points
u11) cd g liq ksp q (sill) - 9 data points
u12) cd g liq ksp q (bi) - 21 data points
u13) bi g liq ksp q (opx) - 6 data points
u14) bi cd g liq ksp q (opx) - 7 data points
u15) cd g opx liq ksp q (bi) - 9 data points
u16) bi g opx liq ksp q (cd) - 4 data points
u17) cd g liq ksp q (opx) - 5 data points
u18) g opx liq ksp q (cd) - 7 data points
u19) g opx liq ksp q (bi) - 11 data points