

Using RBI (read bulk info) tutorial

Richard White.

This is a short tutorial demonstrating the use of the rbi (read bulk info) code in thermocalc to define or change a bulk rock composition. The rbi code allows you to define a bulk rock composition via the mode and composition of phases. One of the more useful applications of this code is to investigate the loss of melt from a bulk rock composition. However, it can also be used to investigate internal buffering of fluids or the fractionation of bulk rock compositions due to porphyroblast growth, at least in a theoretical context. It is also a good way of seeing what the compositions of phases are in oxide mole percent. The rbi code can also be used to reintegrate melt back into a melt depleted rock to make an approximate protolith but this is dealt with in a separate tutorial. In the following sections I highlight several uses for the rbi output

In your THERMOCALC folder you will need the following files

tc-rbi
tc-NCKFMASHp
dr-ml (in whatever folder you have drawpd)

In your tc-prefs file use the scripts;

```
calcmode 1  
scriptfile rbi
```

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

There are two important scripts (in the script file) regarding rbi. The first is

```
printbulkinfo yes
```

What this script does is output a table of modes and mineral compositions in the tc-log file such as the one below.

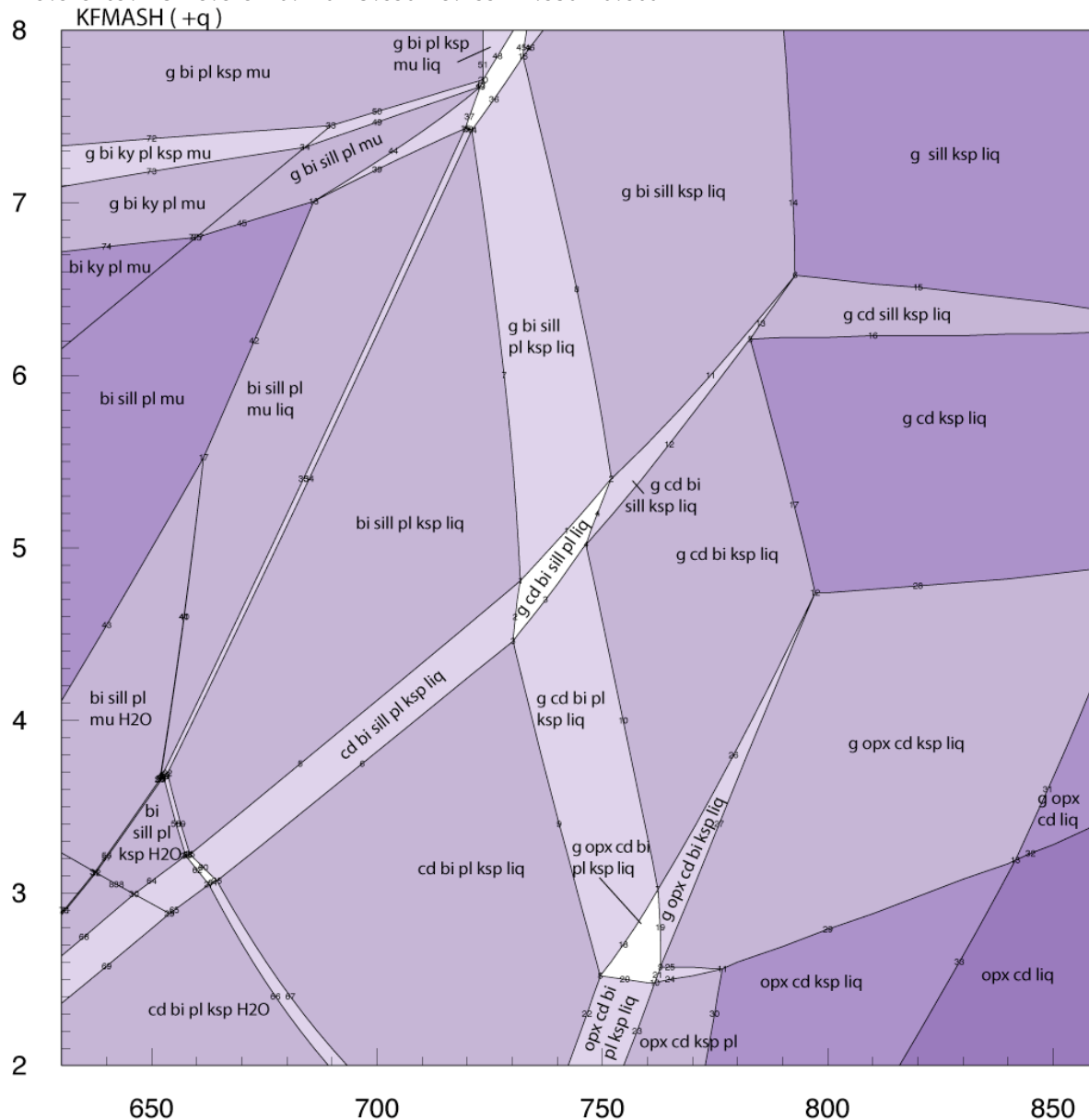
```
% =====  
%          cd          g          liq          ksp          q  
rbi yes  0.128725  0.142898  0.590856          0  0.137521  
  
%          H2O          SiO2          Al2O3          CaO          MgO          FeO          K2O          Na2O  
rbi      0.355525  5.000000  2.000000          0  1.245074  0.754926          0          0  % cd  
rbi          0  3.000000  1.000000  0.021669  0.750962  2.227370          0          0  % g  
rbi      0.320534  2.252573  0.216288  0.012426  0.020572  0.070052  0.149223  0.029450  % liq  
rbi          0  2.993191  0.503404  0.006809          0          0  0.458251  0.038344  % ksp  
rbi          0  1.000000          0          0          0          0          0          0  % q  
% =====
```

This table when pasted into your scripts file is a script that sets the bulk rock composition you are using

In the following section I will use the rbi code to model the loss of melt from a given rock composition. The pseudosection is shown below is that of the basic P-T pseudosection from the first tutorial but extended to higher-P/lower-T and with the muscovite bearing fields and solidus shown.

The bulk composition used is:

H2O	SiO2	Al2O3	CaO	MgO	FeO	K2O	Na2O
5.919	69.113	8.819	0.270	3.590	8.799	2.930	0.560



To remove melt from this composition you must first select the P-T conditions at which to do it. In this example I've picked 5.5 kbar and 800°C which is in the g-cd-ksp-liq-q field. Run thermocalc, for this assemblage and these conditions, setting no phases to zero to get the result

```

P(kbar)    T(?C)    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)
  5.50      800.0    0.3505   0.5604   0.7476  0.01314  0.2147  0.3134   0.2142  0.008712  0.007128  0.7587  0.4383  0.08797  0.004819

mode       cd       g       liq      ksp       q
      0.05619  0.2565  0.3424  0.1199  0.2249

```

this also produces an rbi script in the tc-log file that looks like:

```

% =====
%           cd       g       liq      ksp       q
rbi yes  0.056193  0.256527  0.342443  0.119893  0.224944

%           H2O      SiO2      Al2O3      CaO      MgO      FeO      K2O      Na2O
rbi      0.560410  5.000000  2.000000      0  1.298925  0.701075      0      0  % cd
rbi      0  3.000000  1.000000  0.039410  0.747251  2.213339      0      0  % g
rbi      0.438309  1.858948  0.193909  0.008712  0.006881  0.021633  0.123110  0.033567  % liq
rbi      0  2.995181  0.502409  0.004819      0      0  0.453606  0.043985  % ksp
rbi      0  1.000000      0      0      0      0      0      0  % q
% =====

```

copy and paste this in your script file and turn off the script “setbulkcomp” by putting a % sign in front of it as below:

```

% =====
%           cd       g       liq      ksp       q
rbi yes  0.056193  0.256527  0.342443  0.119893  0.224944

%           H2O      SiO2      Al2O3      CaO      MgO      FeO      K2O      Na2O
rbi      0.560410  5.000000  2.000000      0  1.298925  0.701075      0      0  % cd
rbi      0  3.000000  1.000000  0.039410  0.747251  2.213339      0      0  % g
rbi      0.438309  1.858948  0.193909  0.008712  0.006881  0.021633  0.123110  0.033567  % liq
rbi      0  2.995181  0.502409  0.004819      0      0  0.453606  0.043985  % ksp
rbi      0  1.000000      0      0      0      0      0      0  % q
% =====

```

pseudosection yes

```

% -----
%
% -----
%           H2O      SiO2      Al2O3      CaO      MgO      FeO      K2O      Na2O
%setbulk yes  5.92  69.12  8.82  0.27  3.59  8.80  2.93  0.56
% -----

```

your bulk rock is now set using the rbi script. To remove melt you simply have to change the mode of “liq” in the rbi script. The modes don’t have to add up to 1 as thermocalc will renormalise these. I’m going to change the mode of liq to 3% (i.e. 0.03), though this will be different after the renormalisation. so the mode data in the rbi script should look like:

```

%           cd       g       liq      ksp       q
rbi yes  0.056193  0.256527  0.03  0.119893  0.224944

```

run the same equilibria again at the same P-T conditions and thermocalc will output

```
-----
P(kbar)    T(°C)    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)
  5.50      800.0    0.3505   0.5604   0.7476  0.01314  0.2147   0.3134    0.2142  0.008712 0.007128  0.7587   0.4383   0.08797  0.004819

mode       cd       g       liq       ksp       q
0.08173    0.3731  0.04363  0.1744    0.3272
```

where, after normalisation, the liq proportion is 0.04363. If you really want the normalised proportion to be exactly 0.03 then you can do the maths or take a trial and error approach. In this case to get a normalized result of 0.03 you should change the liq mode to 0.02035 which will return a liq mode of 0.03002. If you want to set it more precisely than this, then you really should seek professional psychological help. For the example here we will run with this more precise mode so your modes in the rbi script should look like:

```
% =====
%
%           cd       g       liq       ksp       q
rbi yes  0.056193  0.256527  0.02035  0.119893  0.224944
```

for this exercise I will continue to use this rbi script to define the bulk rock composition, but you could also run thermocalc and use the bulk rock composition as output during the run, which is now

```
H2O  SiO2  Al2O3  CaO  MgO  FeO  K2O  Na2O
0.976 69.056 9.578 0.244 5.173 12.597 2.143 0.232
```

Notice how, compared with the original bulk, this new one is depleted in water and the alkalis. Silica is much the same as our original bulk had a similar silica content to a melt at these conditions ($\approx 70\%$). If you do use this new output as a bulk composition there may be some small differences due to rounding. Using this rbi composition we would expect much of the lower-T equilibria to change and for the solidus to be elevated. Now you can start to try and calculate the lines around this g-cd-ksp-liq-q field. Starting with the boundary to low T (where bi comes in), this and the other lines that enclose this field still exist but will be in slightly different positions. Where these lines intersect, the lower variance fields can be calculated as well but the (sill) line for g-cd-sill-bi-ksp-liq-q is very short and ends at a (sill liq) point to lower P-T. ie:

```
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)
  6.05      777.1    0.5492   0.5173   0.1037   0.3522   0.6327   0.7623  0.01445  0.1888   0.2934    0.2633  0.008268 0.004012  0.7604   0.4870   0.1027  0.004937

mode       bi       cd       g       liq       ksp       sill       q
0.02318    0.09217  0.3572  0.003158  0.1770    0       0.3473

-----
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)
  6.10      779.0    0.5428   0.5154   0.1051   0.3481   0.6341   0.7579  0.01408  0.1897   0.2933    0.2526  0.008232 0.004073  0.7579   0.4860   0.09800  0.004760

mode       bi       cd       g       liq       ksp       sill       q
0.01554    0.08944  0.3643  0.009364  0.1782    0       0.3432

-----
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)
  6.15      780.8    0.5363   0.5134   0.1064   0.3439   0.6355   0.7536  0.01372  0.1905   0.2934    0.2425  0.008193 0.004132  0.7554   0.4851   0.09370  0.004597

mode       bi       cd       g       liq       ksp       sill       q
0.007920    0.08666  0.3714  0.01562  0.1794    0       0.3390

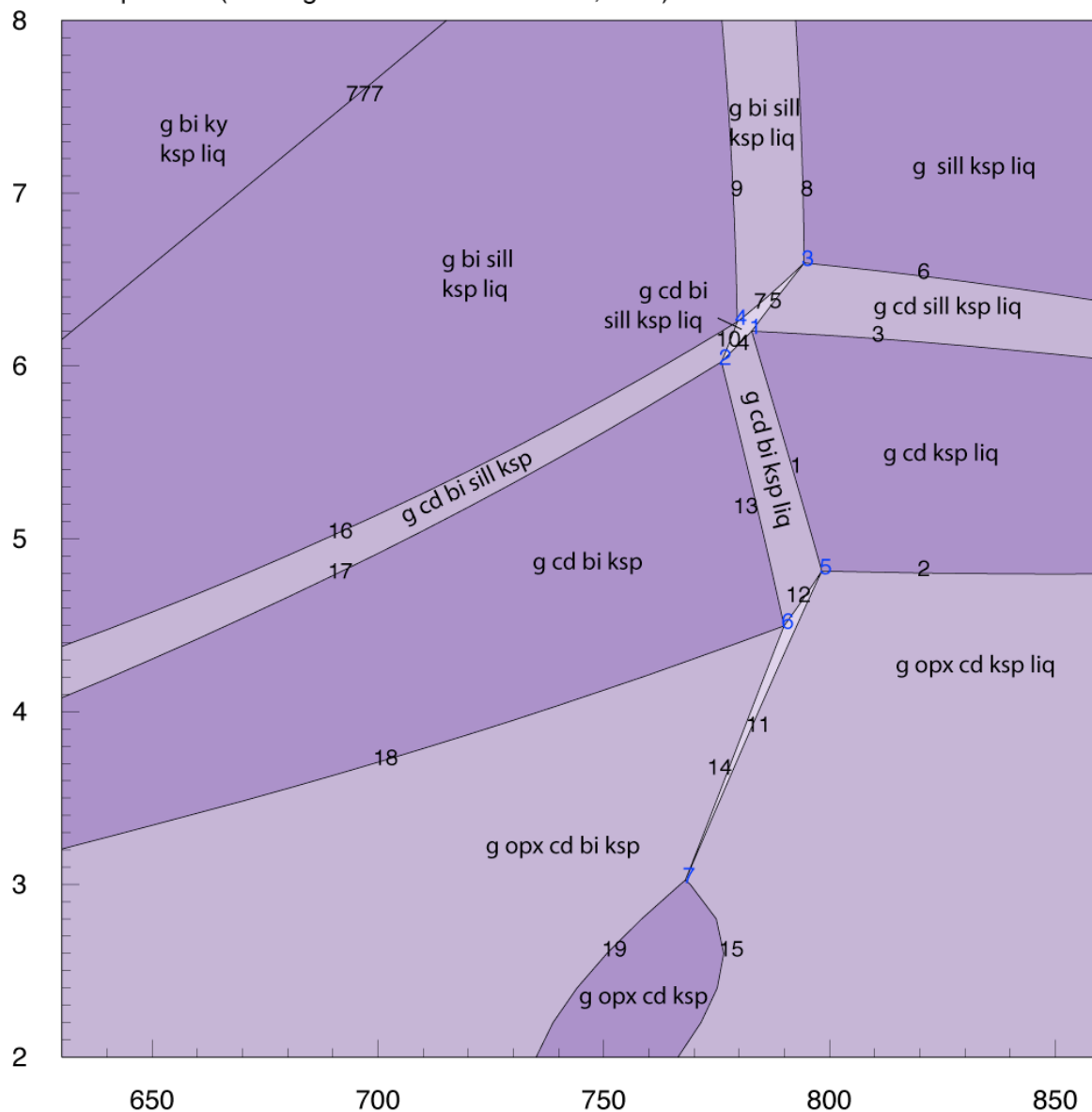
-----
P(kbar)    T(?C)    x(bi)    y(bi)    Q(bi)    x(cd)    h(cd)    x(g)    z(g)    q(L)    fsp(L)    na(L)    an(L)    ol(L)    x(L)    h2o(L)    na(ksp)    ca(ksp)
```

6.20 782.7 0.5298 0.5114 0.1078 0.3398 0.6369 0.7491 0.01338 0.1912 0.2935 0.2330 0.008153 0.004189 0.7529 0.4841 0.08974 0.004447

mode bi cd g liq ksp sill q
 0.0003048 0.08384 0.3785 0.02193 0.1805 0 0.3349

Now that a point where melt runs out is constrained its a matter of calculating the melt-bearing equilibria to higher T and the melt-absent equilibria to lower T. finishing off the pseudosection, it should look like:

drawpd 1.15 (running at 16.45 on Thu 3 Dec,2009)



Example 2: Using rbi to set an appropriate water content at the wet solidus.

For forward modeling partial melting from the wet solidus up T it is important to constrain the water content at the wet solidus such that the assemblages there are just saturated with fluid. The amount of water in the bulk rock required to do this will vary depending on the pressure at which you choose to do this. Starting with the original pseudosection on page 2 you will note that the wet solidus only extends to about 5.5 kbar, thus this bulk rock composition is only appropriate between about 3.6 and 5.5 kbar for modelling rocks that are water saturated at the solidus (below 3.6kbar the water content is too high at the wet solidus due to the subsolidus breakdown of muscovite. The rbi script can be used to set an appropriate water content at a different pressure. If, for example, you want to model this composition crossing the wet solidus at 6.5 kbar then you would have to increase the water content, by just enough to saturate the assemblage at the solidus. Using the original composition, calculate the wet solidus at 5 kbar (ie the assemblage bi-sill-pl-mu-H₂O-liq-q at the (liq) line). The rbi output in the tc-log file should look like:

```
% =====
%          bi      mu      liq      pl      sill      q      H2O
rbi yes  0.380998  0.045327      0  0.054018  0.025023  0.494427  0.000206

%          H2O      SiO2      Al2O3      CaO      MgO      FeO      K2O      Na2O
rbi      1.000000  2.399261  1.100739      0  0.694159  1.705102  0.500000      0  % bi
rbi      1.000000  3.046201  1.453799      0  0.020438  0.025763  0.445699  0.054301  % mu
rbi      0.621608  1.251592  0.133613  0.003012  0.000350  0.001383  0.042921  0.075444  % liq
rbi      0      2.800087  0.599956  0.199913      0      0  0.015555  0.384489  % pl
rbi      0      1.000000  1.000000      0      0      0      0      0  % sill
rbi      0      1.000000      0      0      0      0      0      0  % q
rbi      1.000000      0      0      0      0      0      0      0  % H2O
% =====
```

as in the last example copy & paste this in the script file and turn off the “setbulkcomp” script by putting a % in front of it. Now you need to increase the mode of H₂O in the rbi script. It doesn’t really matter what number you use at this stage as you will need to readjust it at 6.5 kbar, but a increase of a few percent generally does the job. For this exercise I’ve increased it to 5% (ie 0.05) so that the mode info in the rbi script looks like

```
%          bi      mu      liq      pl      sill      q      H2O
rbi yes  0.380998  0.045327      0  0.054018  0.025023  0.494427  0.05
```

now calculate the wet solidus up P from 5kbar to say 7 kbar at 0.1kbar increments. The result for 6.5 kbar is

```
P(kbar)  T(?C)  x(bi)  y(bi)  Q(bi)  fe(mu)  y(mu)  na(mu)  q(L)  fsp(L)  na(L)  an(L)  ol(L)  x(L)  h2o(L)  ca(pl)  k(pl)
6.50     665.3  0.7108  0.5710  0.06679  0.5662  0.9507  0.1452  0.1052  0.2209  0.7391  0.003576  0.0008233  0.8060  0.6637  0.2096  0.02008

mode      bi      mu      liq      pl      sill      q      H2O
0.3597  0.05062      0  0.04908  0.02518  0.4684  0.04704
```

Now we have to reset the H₂O content at 6.5 kbar to the value we want. Typically, given the low porosity of metamorphic rocks we want a number less than 1%, I typically use about 0.4-0.7% (0.004 – 0.007). So get the rbi output in the tc-log file for 6.5 kbar and paste that in your script file. Don’t forget to remove the old rbi script that is already there.

The rbi script will look like:

```
% =====
%          bi      mu      liq      pl      sill      q      H2O
rbi yes  0.359676  0.050620      0  0.049083  0.025184  0.468401  0.047035

%          H2O      SiO2      Al2O3      CaO      MgO      FeO      K2O      Na2O
rbi      1.000000  2.428951  1.071049      0  0.702561  1.726390  0.500000      0 % bi
rbi      1.000000  3.049301  1.450698      0  0.021386  0.027916  0.427409  0.072591 % mu
rbi      0.663708  1.101601  0.123266  0.003576  0.000639  0.002655  0.028823  0.081647 % liq
rbi      0      2.790424  0.604788  0.209576      0      0  0.010040  0.385172 % pl
rbi      0      1.000000  1.000000      0      0      0      0      0 % sill
rbi      0      1.000000      0      0      0      0      0      0 % q
rbi      1.000000      0      0      0      0      0      0      0 % H2O
% =====
```

Now you reset the mode of water to what you want (I'm going with 0.005) and use this as your new bulk rock composition. The mode information in the rbi script will look like:

```
%          bi      mu      liq      pl      sill      q      H2O
rbi yes  0.359676  0.050620      0  0.049083  0.025184  0.468401  0.005
```

running thermocalc again at 6.5 kbar, you output should look like

```
      H2O  SiO2  Al2O3  CaO  MgO  FeO  K2O  Na2O
6.449 68.724  8.769  0.268  3.569  8.750  2.913  0.557
```

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

```
phases : bi, mu, liq, pl, sill, q, H2O
```

```
-----
P(kbar)  T(?C)  x(bi)  y(bi)  Q(bi)  fe(mu)  y(mu)  na(mu)  q(L)  fsp(L)  na(L)  an(L)  ol(L)  x(L)  h2o(L)  ca(pl)  k(pl)
6.50     665.3  0.7108  0.5710  0.06679  0.5662  0.9507  0.1452  0.1052  0.2209  0.7391  0.003576  0.0008233  0.8060  0.6637  0.2096  0.02008

mode      bi      mu      liq      pl      sill      q      H2O
0.3755  0.05284      0  0.05124  0.02629  0.4890  0.005219
```

Again, its up to you if you want to calculate the rest of the diagram with the bulk rock defined via the rbi script or use the output mol% oxide bulk given by thermocalc. You could now calculate the rest of the wet solidus to higher pressures, though I won't go through that here.

There are a number of other uses for the rbi script.

- 1) you can use this script for modeling fractionation of, say, garnet from the bulk
- 2) you can use this to create an approximate "protolith" composition from a melt depleted bulk by re-integrating melt back into the bulk composition (this will be a separate tutorial)
- 3) the rbi script is a good way of constructing the actual composition of phases for easy comparison with probe data for example as each phase composition is given as oxide moles