A quick start guide to performing calculations on melting in THERMOCALC

This guide is intended to help the reader to perform calculations if they are not familiar with THERMOCALC. More detailed documentation and tutorials for using THERMOCALC can be found at http://www.metamorph.geo.uni-mainz.de/THERMOCALC/. Instructions are for use in OSX and Linux.

Part 1: Drawing the PT pseudosection for RE46 icelandic basalt

1) Download the program and input files

Download these from the supplementary material:

```
tc-ds633.txt          # internally-consistent dataset updated with the end-members used
tc-KNCFMASTOCr.txt    # a-x file (activity-composition models)
tc-bas.txt            # THERMOCALC input scripts file
tc-prefs.txt          # THERMOCALC preferences file
```

Download the most recent version of THERMOCALC here: http://www.metamorph.geo.uni-mainz.de/THERMOCALC/getstarted/index.html

Put them all in the same folder.

2) The tc-bas file

This input file is the only one that needs adjusting for the purpose of performing simple calculations. It contains information about settings for calculations and output required, starting guesses and the bulk composition. The bulk composition *must* be given in mol%. Information below the * is not read; here you will find a range of useful starting guesses, and can add your own as they are generated. These can simply be copied and pasted over the starting guess near the start of the file. Anything after a % on a line is ignored and is useful for comments.

The starting guesses initially provided in this file work for all of the *PT* space. New starting guesses are generated with each calculation in the tc-log.txt file. If, in other calculations, the program no longer finds a solution where there should be one, a starting guess at closer *PT* conditions to those required could be pasted in from the log file.

3) Running THERMOCALC and calculating an invariant point.

Here we will calculate the position of the inflection point on the liquidus where liq coexists with ol and cpx, see the red spot on the diagram below. Univariant lines and invariant points are located by finding the position where one or more phase modes become zero.

Open the terminal and navigate to the folder where the above files are saved. Type:

```
./tc347               # or which ever version you are using. This runs the program.
```

Below is an example run: Replies to THERMOCALC prompts are in red, comments in blue}

```
THERMOCALC 3.46 (Free Pascal version)

calculation type :
     0 = table of thermodynamic data of end-members
     1 = phase diagram calculations
     2 = average pressure-temperature calculations
     3 = calculations on all reactions between end-members
     4 = list end-member names and compositions
control code  : 1                              {for phase diagram calculations}
```

```
suffix to name for script info datafile : bas    {for input file tc-bas.txt}
the main output is in the file, "tc-bas-o.txt"
other (eg drawpd) output is in the file, "tc-bas-dr.txt"

    1.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00
    0.00    1.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00
    0.00    0.00    1.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00
    0.00    0.00    0.00    1.00    0.00    0.00    0.00    0.00    0.00    0.00
    0.00    0.00    0.00    0.00    1.00    0.00    0.00    0.00    0.00    0.00
    0.00    0.00    0.00    0.00    0.00    1.00    0.00    0.00    0.00    0.00
    0.00    0.00    0.00    0.00    0.00    0.00    1.00    0.00    0.00    0.00
    0.00    0.00    0.00    0.00    0.00    0.00    0.00    1.00    0.00    0.00
    0.00    0.00    0.00    0.00    2.00    0.00    0.00    0.00    1.00    0.00
    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    1.00

^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^

THERMOCALC running at 10.47 on Wed 18 Feb,2018
using tc-ds633.txt produced at 20.37 on Fri 23 Jun,2017 (sigfit =  1.048)
with axfile tc-KNCFMASTOCr.txt and scriptfile tc-bas.txt

liq  pl  plc  spn  cm  g  ol  opx  cpx  pig  ilm  ksp
choose from: liq  pl  plc  spn  cm  g  ol  opx  cpx  pig  ilm  ksp
which phases : ol cpx liq                    {enter all phases involved, including liq}
no phases in excess (from script)
variance of required equilibrium (9?) : y    {or just hit return for default answer}
set mode isopleths ? y                       {or just hit return, to set modes of phases}
set modes to zero (to find edges/corners of fields) ? y     {or just hit return}
you may set zero modal proportions, from: liq ol cpx
which to set : cpx ol                        {phases whose modes to be set to zero}

specification of PT window:
PT window within which invariant points expected to lie
T low,high, P low,high : 1200 1300 4 6     {or hit return if ranges are already provided in tc-bas.txt}
composition (from script)
   SiO2  Al2O3    CaO    MgO    FeO    K2O   Na2O   TiO2      O  Cr2O3
 49.791  9.260 14.760 16.272  7.599  0.010  1.532  0.378  0.378  0.020
<================================================>
phases : liq ol cpx

-------------------------------------------------------------------
 P(kbar)     T(°C)     wo(L)     sl(L)     fo(L)     fa(L)     jd(L)
  5.2857  1255.733    0.4228    0.2211    0.1165   0.04900   0.08775
                      o(cpx)    n(cpx)    Q(cpx)    f(cpx)   cr(cpx)
                      0.2697   0.01507  -0.03256   0.01595  0.009758
               SiO2  Al2O3    CaO    MgO    FeO    K2O   Na2O   TiO2
             49.791  9.260 14.760 16.272  7.599  0.010  1.532  0.378

    mode       liq        ol       cpx          G
           1.000         0         0 -993.51919

more phase diagram calculations ? n          {or hit return for a new calculation}
================================================
all done - hit return to exit ?              {hit return}
```

The results appear in the terminal. The *P* and *T* of the point are given, along with the phase compositions (look at tc-KNCFMASTOCr.txt to find out what they mean. For example, x(ol) = fayalite content of olivine. Finally, the liquid composition is given, first in mol% with FeO and O,

secondly in mol% with FeO and Fe_2O_3, thirdly in wt.% with FeO and Fe_2O_3, as illustrated below:

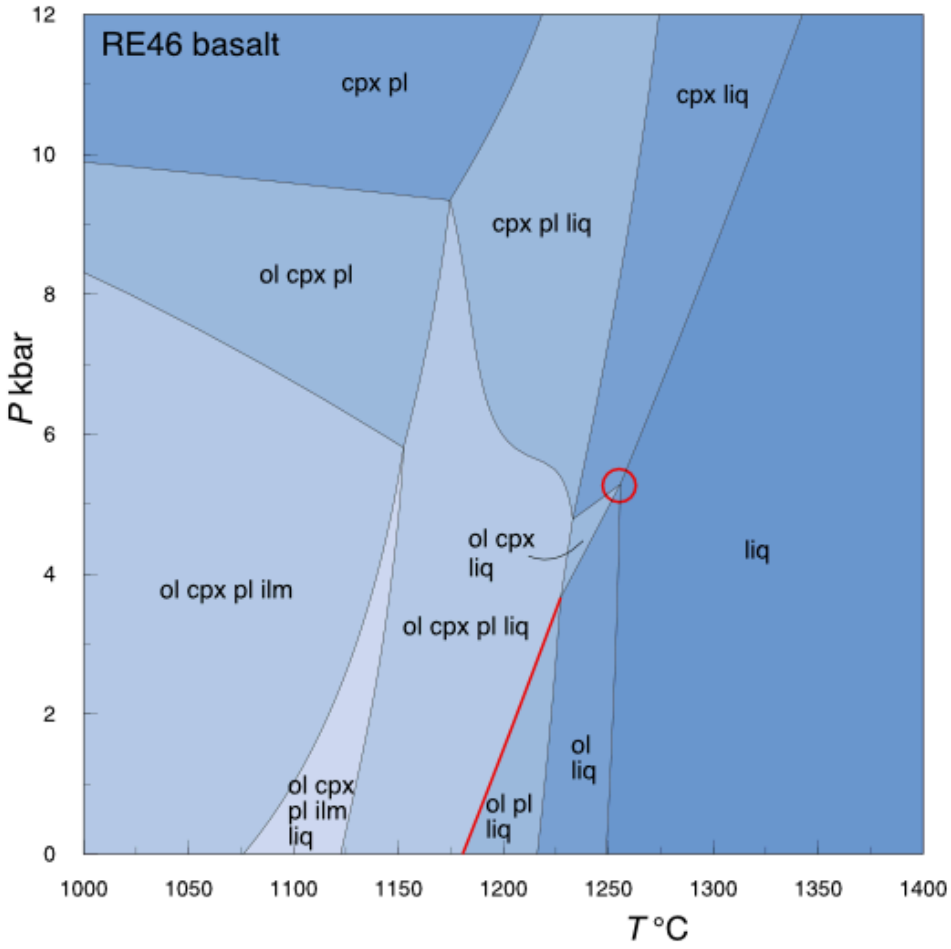
```
   SiO2  Al2O3    CaO    MgO    FeO    K2O    Na2O   TiO2      O  Cr2O3
 49.791  9.260 14.760 16.272  7.599  0.010  1.532  0.378  0.378  0.020  ==>

      1      2      3      4      5      6      7      8      9     10
  50.17   9.33  14.87  16.40   6.90   0.01   1.54   0.38   0.38   0.02  ==>

      1      2      3      4      5      6      7      8      9     10
  49.04  15.48  13.57  10.75   8.06   0.02   1.56   0.49   0.99   0.05
```

The full output is also printed to the file tc-bas-o.txt, and new starting guesses and other information are generated in tc-log.txt.

For convenience, a brief version of the results containing just *P*, *T* and liquid composition in wt.% appear in the file tc-bas-dr.txt. These can be copied into an input file to use with the program drawpd, or read in to a different plotting program.



4) *Calculating a univariant line*

A univariant line (field boundary with one phase added/lost) can be calculated as above, but by giving just a single phase to set to zero.

To find the line for the assemblage ol cpx pl liq where cpx disappears (as in red line above), run THERMOCALC as above, but change responses as below:

```
control code  : 1                                  {for phase diagram calculations}
suffix to name for script info datafile : bas      {for input file tc-bas.txt }
…
liq  pl  plc  spn  cm  g  ol  opx  cpx  pig  ilm  ksp
```

```
choose from: liq  pl  plc  spn  cm  g  ol  opx  cpx  pig  ilm  ksp
which phases : ol cpx pl liq                    {list of phases to consider}
no phases in excess (from script)
variance of required equilibrium (8?) :              {hit return}
you may set zero modal proportions, from: liq pl ol cpx
which to set : cpx
calculate T at  P (rather than P at T) ?  y          {or hit return, for getting T at known P's}

specification of PT window:
P range over which T of reactions to be calculated  {hit return, or enter Pmin, Pmax in kbar}
P window: P low,high : 0.001 4                      {we want results from 0 to 4 kbar}
T window within which reactions expected to lie?
T window: T low,high :                              {hit return, or enter Tmin Tmax in °C}
P window :0.001 <-> 4 kbar :P interval : 0.5        {want results every 0.5 kbar}
```

The solutions quickly appear in the terminal, along with the same output files as described above.

You should now be able to calculate a complete *PT* pseudosection.

5) *Hints and tips*

- Metastability: THERMOCALC doesn't know if an assemblage is metastable. For example, the above line could not be calculated to, say, 5 kbar, because it projects into a field of higher variance (fewer phases) and one phase (pl) has gone to zero above 4 kbar in the field ol cpx liq. However, the line (ol liq -pl) where pl goes out in the assemblage ol pl liq can be found at higher pressures, as this assemblage is a subset of the assemblage ol cpx pl liq into which the line projects metastably. Similarly, subsolidus phase boundaries can be incorrectly calculated at temperatures above the solidus. Pay close attention to geometry around invariant points. Where 4 fields meet at a point the assemblages contain *n*, *n*+1, *n*+2, *n*+1, and back to *n* phases going around the point.
- If no solutions appear, try changing the starting guesses.
- For pretty plots formatted as they are in this study, use the program drawpd.

Part 2: Other types of diagram

Detailed help with these can be found at http://www.metamorph.geo.uni-mainz.de/THERMOCALC/

1) *PX pseudosections*

Isothermal *PX* pseudosections investigate the effects of changing bulk composition on the location of phase boundaries. Isobaric *TX* plots could also be generated. A complete tutorial for how to do this can be found on the THERMOCALC website.

2) *Isopleths*

Isopleths of constant phase mode can be easily tracked by setting the mode to a value greater than 0. Isopleths of constant phase composition can be calculated by first editing the following line in the input file:

setiso no → setiso yes or → setiso ask

The list of phase composition variables can be seen in the starting guesses or in the file tc-KNCFMASTOCr.txt. The terminal interactive instructions should be self-explanatory. Again, beware of metastable extensions of lines. See the THERMOCALC website for more help.