

A quick start guide to performing calculations on peridotite melting in THERMOCALC

This guide is intended to help the reader to recreate the calculations performed in this study 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, and after the program has started up, they are also applicable to Windows.

Part 1: Drawing the PT pseudosection

1) Download the program and input files

Download these from the supplementary material:

tc-ds622.txt # internally-consistent dataset updated with the end-members used in this study
tc-NCFMASCrO.txt # a-x file (activity-composition models)
tc-kh.txt # THERMOCALC input scripts file
tc-prefs.txt # THERMOCALC preferences file

Download the most recent version of THERMOCALC here:

<http://www.esc.cam.ac.uk/research/research-groups/holland/thermocalc/thermocalc-2013-dataset>
Version 336 or above is required.

Put them all in the same folder.

2) The tc-kh file

This input file is the only one that needs adjusting for the purpose of performing the calculations in this study. 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.

The starting guess initially provided at the top of this file is for $liq = 0$, $g = 0$. This is the invariant point where the garnet-out boundary intersects the solidus; from here, much of the PT space is accessible, including the whole solidus. New starting guesses are generated with each calculation in the -log.txt file. If the program no longer finds a solution where there should be one, a starting guess at closer PT conditions to those required could be used.

3) Running THERMOCALC and calculating an invariant point.

Here we will calculate the position of the spinel-out – solidus intersection (the $liq=0$ $sp=0$ invariant point), 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:

`./tc337` # 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 3.40 (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 : kh {for input file tc-kh.txt}
the main output is in the file, "tc-kh-o.txt"
other (eg drawpd) output is in the file, "tc-kh-dr.txt"


    1.00      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      1.00      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      1.00      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      1.00      0.00
    0.00      0.00      0.00      0.00      0.00      0.00      0.00      1.00

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

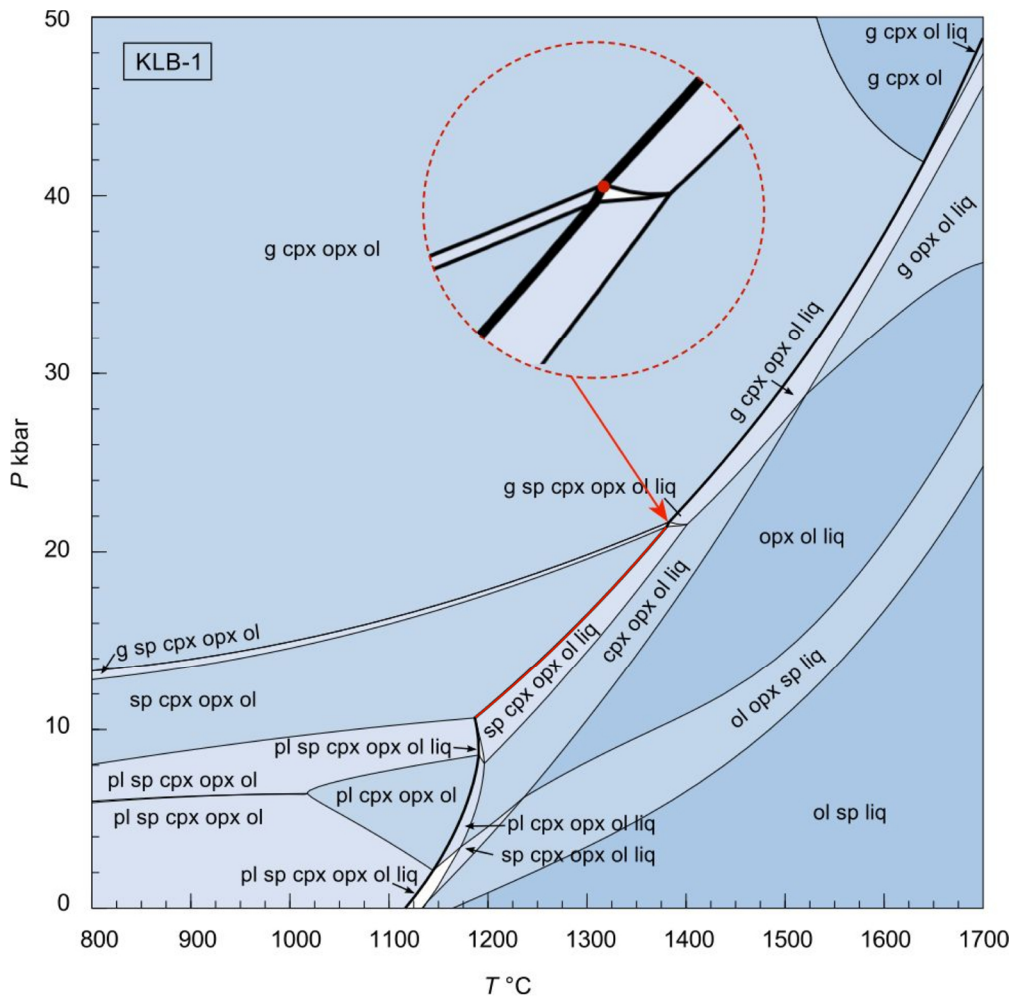
THERMOCALC running at 10.47 on Wed 18 Feb,2015
using tc-ds63.txt produced at 15.31 on Sat 24 Jan,2015 (sigfit = 1.033)
with axfile tc-NCFMASCrO.txt and scriptfile tc-kh.txt


liq pl cpx ol sp cm g opx
choose from: liq pl cpx ol sp cm g opx
which phases : ol cpx opx sp g liq {enter all phases involved, including sp & liq}
no phases in excess (from script)
variance of required equilibrium (4?) : 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 cpx ol sp g opx
which to set : liq sp {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 : 1000 1600 10 40 {or hit return if ranges are already provided in tc-kh.txt}
composition (from script)
   SiO2 Al2O3 CaO MgO FeO Na2O O Cr2O3
  38.494 1.776 2.824 50.565 5.886 0.250 0.096 0.109
<=====>
phases : liq cpx ol sp g opx


-----
P(kbar)       T(?C)         ct(L)          jd(L)          di(L)          fa(L)          fo(L) ...
21.6800     1383.087        0.1884         0.2304         0.1797         0.1051         0.1855 ...
                                   ek(L)          x(cpx)         y(cpx)         o(cpx)         n(cpx) ...

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



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 solidus line for the assemblage ol cpx opx sp (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 : kh      {for input file tc-kh.txt }
...
liq pl cpx ol sp cm g opx
choose from: liq pl cpx ol sp cm g opx
which phases : ol opx cpx sp liq                {list of phases to consider}
no phases in excess (from script)
variance of required equilibrium (5?) :          {hit return}
you may set zero modal proportions, from: liq cpx ol sp opx
which to set : liq
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 : 11 21                     {we want results from 11 to 21 kbar}
T window within which reactions expected to lie?
T window: T low,high :                            {hit return, or enter Tmin Tmax in °C}
P window :11 <-> 21 kbar :P interval : 1         {want results every 1 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 be calculated to, say, 25 kbar, without problem, though the answer would not be correct as garnet comes into the assemblage - pay close attention to geometry around invariant points. Also, a low variance (more phases) line will not continue metastably into a higher variance (fewer phases) field. So, the line (cpx opx ol sp g -liq; solidus in a garnet spinel lherzolite) cannot be accidentally calculated to higher or lower pressures, as the fields above and below are higher variance and cannot contain all of these phases. However, the line (cpx opx ol sp g -liq) can be found at higher pressures, as this assemblage is a subset of cpx opx ol sp g liq. Similarly, subsolidus phase boundaries can be incorrectly calculated at temperatures above the solidus. Try to calculate boundaries involving the most phases first to keep things simple.
- If no solutions appear, try a closer starting guess. This point can be generated anywhere – not just on an invariant point.
- 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 (fig. 3) 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.

The input file (tc-kh.txt) must be edited. Replace the bulk composition with the following two lines:

```
setbulk yes 38.494 1.776 2.824 50.566 5.886 0.250 0.096 0.0 % KLB-1 X=0
setbulk yes 38.494 1.776 2.824 50.566 5.886 0.250 0.096 2.0 % KLB-1 X=1
```

We can now calculate linear mixtures of these two compositional end-members. X=0 uses the first bulk composition, X=1 the second, X=0.5 uses half of each etc. Here we are varying the proportion of Cr₂O₃ from 0 mol.% to 2 mol.% while keeping other components constant (subject to renormalisation to 100%). THERMOCALC 'sees' the two bulk compositions and adjusts the instructions accordingly; these instructions are self-explanatory. Invariant points are trickier to deal with in this mode as two phases cannot be specified to equal 0 at a fixed *P* or *T*, so look for where lines intersect or where low variance lines terminate (see the website tutorials).

2) Isopleths

Isopleths of constant phase mode (e.g. fig. 4c and 4d) can be easily tracked by setting the mode to a value greater than 0. Isopleths of constant phase composition (e.g. fig. 4a and 4b) 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-NCFMASCrO.txt. The terminal interactive instructions should be self explanatory. Again, beware of metastable extensions of lines.