New Melt Model – some notes

The folder for mac & linux has unix line-ending files and the folder for windows contains windows line-ending files. Otherwise they are identical.

1. The model uses the newest THERMOCALC (tc350) from the website at https://hpxeosandthermocalc.org. Thus it requires files set up according to the new prescriptions given in the documentation in the download of tc350.

2. Quick start:

   Unless you are very familiar and confident, make a copy of the folder KR4003 and use the copy for experimenting at first. Run THERMOCALC from the commandline (mac, win, or linux). To calculate the invariant point at 14.2 kbar and 1369°C involving ol + cpx + opx + spn + liq where both spn and cpx simultaneously disappear, enter the names of the 5 phases when prompted. Set cpx and spn modes to zero when prompted and THERMOCALC will print out the $P\&T$ as well as the calculated compositions of all phases. Follow the example log file (kr4003_eg_log.txt) as a guide if you are new to using THERMOCALC.

3. The folder provided here includes all files required for building the KR4003 pseudosection of Figure 1 in Tomlinson & Holland (2021). These are as follows:

   - tc-ds634.txt

     The updated Holland & Powell thermodynamic dataset modified to include the changes made for Tomlinson & Holland (2021).

   - tc-KNCFMASTOCr.txt

     The model activity-composition file corresponding to the phases involved.

   - tc-kr4003.txt

     The script file for setting up calculations for peridotites such as KR4003.

   - tc-prefs.txt

     The standard prefs file which tells THERMOCALC where to look for a script.

4. Output files: tc-kr4003-o.txt is the standard output file containing the calculated results. tc-kr4003-dr.txt is the output in a form that can be pasted into a drawpd file

to make a drawing. tc-log.txt is the generated log file and contains much useful information such as starting guesses generated from the calculated results and phase compositions in more human-readable form. Further information may be found in

– tc-xxx-it.txt: more humanly readable version of the activity models used

– tc-xxx-ic.txt: much more information including mineral compositions, site-fractions, bulk density etc

– tc-xxx-csv: comma separated file of PT output

5. Drawing a pseudosection.

   This involves building up a drawpd file such as the example dr-kr4003.txt. This example contains all the data needed to draw the *PT* pseudosection for KR4003. Just run the program dr118, after setting the filename kr4003 in the dr-prefs file, and an eps file is produced which can be labelled and annotated or edited in a drawing package such as Illustrator, Inkscape, or Affinity Designer. A fully annotated pseudosection is provided as file KR4003.pdf which is a tidied up version of the automatically produced dr-kr4003.eps.

   An analogous folder is provided for sample BP002. Here the opx uses a different variable a(opx) rather than y(opx) to make calculation of isopleths easier for total Al in opx (a(opx)). Here a(opx) $= 4X^T_{Al} - X^{M1}_{Cr} - X^{M1}_{Fe3} + X^{M2}_{Na} - 2X^{M1}_{Ti}$ is used in place of the variable y(opx) $= 2X^T_{Al}$ as in files in the KR4003 folder. Both formulations yield exactly the same calculated results.

   BP002 is assumed K_2O-free and so initial guesses for K-variables are set to zero, boiling the system down to NCFMASTOCr.

6. Where next?

   If you are new to THERMOCALC then there is a wealth of information including documentation as well as tutorials at the website https://hpxeosandthermocalc.org.