Practical: Mineralogical Earth Models with HeFESTo

We will use the principles of thermodynamics combined with semi-empirical thermodynamic models of mantle phases, as embodied in the code HeFESTo, to explore mineralogical models of Earth's mantle. The purpose is to introduce you to thermodynamic concepts and to explore the relationship between the properties of minerals, mineral assemblages (rocks), and Earth. We will be focusing on the upper 800 km because this region is where our knowledge is most secure.

Much of the foundation is given in *Stixrude & Lithgow-Bertelloni* (2005,2011). Some applications are discussed in *Xu et al.* (2008) and *Stixrude & Lithgow-Bertelloni* (2012). Briefly the code computes for a given pressure, temperature, and bulk composition, i) the stable phase assemblage, including the abundances and compositions of the phases coexisting in equilibrium ii) the physical properties of those phases iii) the physical properties of the multi-phase assemblage and iv) scaling of physical properties to seismological time scales.

What do you need to know about running HeFESTo? The input file that we will be playing with is:

control – specifies the bulk composition, range of P/T, superadiabatic temperature, and the set of mantle phases and species (end-members) to be included in the minimization.

There are many output files of which two will be most useful for this exercise:

fort.59 – Some physical properties of the assemblage
fort.66 – Relative amounts of phases

I have also prepared a number of scripts to assist in analyzing the results.

1. Baseline case. Compute the phase equilibria and density of pyrolite along the 1600 K isentrope. The control file is already set up for this case, as is the isentropic temperature profile along which the entropy is constant.

    a) Examine the physical properties profiles. Identify depths at which the physical properties change rapidly (discontinuities). See if you can guess what some of these are caused by before going on.
    b) Examine the phase equilibria. The plot shows the amount of each phase as a function of depth. Identify each density anomaly with a change in phase assemblage.
    c) Question. Which of the density anomalies that you identified can be associated with seismic discontinuities or other anomalies that have been found in the mantle? Which seismologically identified mantle discontinuities do not show up in your calculation?

2. Thermally perturbed case. The last entry of the first line of the control file is the superadiabatic temperature. For the baseline case, this was set to 0. Change it! I would suggest a value of -200, corresponding to 200 K subadiabatic temperature.

    a) Compare the density profiles of cold and baseline cases. Does the density change with temperature by approximately the same amount at all depths? Rationalize the results by examining the phase equilibria.
    b) What might be the dynamical significance of large variations in the effect of temperature on density, i.e. the thermal expansivity?
    c) How has the discontinuity structure changed?

3. Compositionally perturbed case. Change the superadiabatic temperature back to 0. The second column of lines 4-9 specify the bulk composition. For the baseline case, these were set to the depleted MORB mantle of *Workman and Hart*, 2005. Explore the influence of compositional perturbations by changing these entries. I would suggest initially trying the MB Mars composition of *Bertka and Fei* (1997). The largest difference to pyrolite is Fe enrichment at the expense of Mg.

    a) Compare the velocity profiles of compositionally perturbed and baseline cases. Does the velocity change in the same direction at all depths? Rationalize the results by examining the phase equilibria.
    b) How does the magnitude of the changes caused by thermal and compositional perturbations compare with the magnitude of lateral heterogeneity seen in seismic tomography?
    c) How has the discontinuity structure changed?

References

Bertka, C. M. and Y. Fei, Mineralogy of the Martian interior up to core-mantle boundary pressures, *Journal of Geophysical Research, 102*, 5251-5264, 1997.

Stixrude, L. and C. Lithgow-Bertelloni, Thermodynamics of mantle minerals: 1. Physical properties, *Geophysical Journal International*, *162*, 610-632, doi: 10.1111/j.1365-246X.2005.02642.x , 2005.

Stixrude, L. and C. Lithgow-Bertelloni, Thermodynamics of mantle minerals II, Phase equilibria, *Geophysical Journal International, 184*, 1180-1213, 2011.

Stixrude, L. and C. Lithgow-Bertelloni, Geophysics of chemical heterogeneity in the mantle, *Annual Reviews of Earth and Planetary Sciences, 40*, 569-595, doi: 10.1146/annurev.earth.36.031207.124244, 2012.

Workman, R. K., and S. R. Hart (2005), Major and trace element composition of the depleted MORB mantle (DMM), *Earth And Planetary Science Letters*, *231*, 53-72.

Xu, W., C. Lithgow-Bertelloni, L. Stixrude, and J. Ritsema, The effect of bulk composition and temperature on mantle seismic structure, *Earth and Planetary Science Letters, 275*, 70-79 doi:10.1016/j.epsl.2008.08.012, 2008.

Structure of control file.

- Line 1.

First pressure, last pressure, number of pressure intervals, first temperature, last temperature, number of temperature intervals, super-adiabatic temperature

Note that by entering -1 for the number of temperature intervals, the code reads in the temperature profile from the file “ad.in”. In this case, the entries for first temperature and last temperature are not used.

- Line 2.

Number of components, *c*. Further entries are not used.

- Line 3.

Specifies that all components are oxides. Should not be changed.

- Lines 4 to 4+*c*-1.

Name of component, amount of component. Further entries not normally used.

Name of component is specified by the chemical symbol of the cation.

Amounts are specified in mole fraction of the oxide on a single cation basis (e.g. SiO_2, $AlO_{1.5}$)

- Line 4+c

Level of theory. Don’t change

- Line 4+c+1

Number of end-member species

- Remaining lines

These specify the phases to be included; a code to indicate whether they are present (1) or not (0) in the initial guess; and the names of the end-member species to be included for that phase. Note that the initial guess must span the bulk composition.

Editing a file.

The easiest way is with “vi” i.e. “visual editor”.

- Open a file in vi
%vi file_name

- Quit an editing session

Without saving
:q

Saving changes
:wq

- Moving around the file
h,j,k,l

move respectively: left, down, up, right

- Delete a character
x

- Input text
i
enter desired text
esc

- Start entering text on a new line below the cursor
o
Enter desired text
esc

- Start entering text on a new line above the cursor
O
Enter desired text
esc

- Much more information about vi is available on the web; e.g.

http://docs.freebsd.org/44doc/usd/12.vi/paper.html