EARTH 438 - Advanced Topics in Geophysics (C.R. Bina, 2017)

Basic Exercises in the Use of the Perple_X Code
(cf. Connolly, 1990, 2005, 2009; Connolly and Kerrick, 1987; Connolly and Petrini, 2002; etc.)

exercises version 2017-11-18-crb

Installation

Install the Perple_X software (current version 6.7.9 or 6.8.0) on your computer. Note that this is old-school software, largely command-line driven without graphical user interfaces.

- Linux executables available as gzipped tar file here;
- Mac executables available as zip file here;
- Windows executables available as zip file here;
- Data files available as zip file here;
- Fortran sources (not necessary - only for the curious) available here.

Perple_X Example 1 (Earth 438, C.R. Bina, 2017)

After installing Perple_X:

1) Use "build" to construct an input file for the following simple problem.

- thermodynamic data file: stx11ver.dat
- computational option file: accept default
- transform components: no
- saturated components: no
- chemical potentials as independent variables: no
- select components: MGO, SIO2
- computational mode: accept default
- dependent potentials: no
- x-axis: P (range: 1 to 3e+05 bar)
- T range: 300 to 2300 K
- specify by weight: no
- molar composition: 100% Mg2SiO4
- print file: yes
- exclude pure phases: no
- include solution models: no

2) Use "vertex" to find equilibrium by free-energy minimization.

3) Use "pssect" to plot the resulting P-T section. View and print the PostScript file.

How do your results compare to Figure 6 of Stixrude and Lithgow-Bertelloni (2011)? How do they compare to the ancient Figure 1a of Bina and Liu (1995)?

4) Use "werami" to find the following properties at conditions of (230 kbar, 2000 K) and at conditions of (240 kbar, 2000 K).

- phases present and their relative proportions by volume
- compositions of each of the phases present
- density of the assemblage
- Poisson's ratio for the assemblage

Perple_X Example 2 (Earth 438, C.R. Bina, 2017)

1) Use "build" to construct an input file for the following slightly less simple problem.

- select components: MGO, SIO2, FEO
- molar composition: 90% Mg2SiO4 + 10% Fe2SiO4
- include solution models: yes
- solution model file: stx11_solution_model.dat
- select solution models: O, Wad, Ring, Wus, Aki, Pv

2) Use "vertex" to find equilibrium by free-energy minimization.

3) Use "pssect" to plot the resulting P-T section. View and print the PostScript file.

How do your results compare to the ancient Figure 1b of Bina and Liu (1995) or to the even older Figure 1 of Ita and Stixrude (1992)?

4) Use "werami" to find the following properties at conditions of (230 kbar, 2000 K) and (240 kbar, 2000 K).

- phases present and their relative proportions by volume
- compositions of each of the phases present
- density of the assemblage
- Poisson's ratio for the assemblage

5) Answer the following question, based on your results. When the phases ferromagnesian silicate perovskite (bridgmanite) and magnesiowüstite (ferropericlase) coexist in equilibrium, into which phase does iron partition more strongly?

Perple_X Example 3 (Earth 438, C.R. Bina, 2017)

Starting from your successful results in Example 2, modify it to approximate a case in which olivine persists metastably, so that wadsleyite never forms. To do this, you will need to add both "wad" and "fwad" to the "excluded phase list". You can accomplish this simply by running "build" again, or (if you are feeling brave) you can just use a text editor to edit a copy of "example2.dat" to produce a suitable "example3.dat" file.

Answer the following questions, based on your results, by comparing the phase diagram for example 3 with that from example 2.

1. What happens to the ringwoodite field at low temperatures?
2. What happens to the ringwoodite field at high temperatures?
3. What happens to the olivine field at low temperatures?
4. What happens to the olivine field at high temperatures?
5. Examine question 4 in detail by using "werami" to compare the phase assemblages at (145 kbar, 1900 K) for example 3 vs. example 2.

How do your results compare to Figure 9 of Walton et al. (2014)?

Perple_X Example 4 (Earth 438, C.R. Bina, 2017)

You will now pursue a model similar to Example 2, except that you will seek to create a P-X diagram instead of a P-T diagram. For the bulk compositions, instead of an Fo_{90} olivine composition, however, you will return to the eclogite-garnetite transition whereby enstatite dissolves into pyrope to form a garnet-majorite solid solution. You should run "build" again, to create a suitable "example4.dat" file.

Your instructions to "build" will be similar to those in Example 2, except for the following major changes.

- The chemical components needed are MGO, SIO2, and AL2O3.
- The x-axis variable will be option 3: "Composition X(C1)* (user defined)".
- The y-axis variable will be P, with a range of 1 bar to 220 kbar.
- Temperature will be fixed at 1300 K.
- Compositions along the x-axis will range from C0=$Mg_4Si_4O_{12}$ to C1=$Mg_3Al_2Si_3O_{12}$.
- You need to include the following solution models: Opx, Aki, Gt.

Plot the resulting P-X phase diagram.

How do your results compare to Figure 6 of Zhang and Liou (2003)? How do they compare to the ancient Figure 1a of Bina and Wood (1984) or to its precursor Figure 3 of Akaogi and Akimoto (1977) recently reprinted as Figure 4 of Akaogi (2016)?

After you are convinced that you have constructed the correct phase diagram, if you are feeling ambitious, you can try to improve the resolution of your phase boundaries by changing some of the Perple_X options from their default values in the "perplex_option.dat" file. Some values that I have found useful for such purposes include:

- auto_refine_factor_I → 6
- auto_refine_factor_II → 8
- final_resolution → 1.0e-4 1.0e-4
- initial_resolution → 1/30
- solvus_tolerance_II → 0.1

PerpleX Example 5 (Earth 438, C.R. Bina, 2017)

You will now pursue another model similar to Example 2, except that you will use a more complex composition. The "pyrolite" model is a family of compositions initially proposed by [Ringwood (1962)](#) as a likely composition for Earth's upper mantle, consisting of roughly one part basalt to four parts dunite. (The name is derived from **pyr**oxene and **ol**ivine.) There are many different estimates of "pyrolite" compositions. You will use one devised by [Stixrude and Lithgow-Bertelloni (2005)](#) ("Pyrolite" from their Table 1) as a highly simplified version of a composition proposed by [Ringwood (1979)](#).

Your instructions to "build" will be similar to those in Example 2, except for the following changes.

- The chemical components needed are SIO2, MGO, FEO, CAO, and AL2O3. (For brevity, NAO was neglected while simplifying this particular "pyrolite" model.)
- The x-axis variable will be P, with a range of 1 bar to 300 kbar.
- The y-axis variable will be T, with a range of 300 K to 2800 K.
- You will include all of the solution models offered, with one exception. For garnet-majorite, you will choose the full Gt_maj solution, ignoring both the simpler Gt and Gt_cmaj solutions.

Use "pssect" to plot the resulting P-T phase diagram.

How do your results compare to Figure 16 of [Stixrude and Lithgow-Bertelloni (2011)](#)?

Answer the following questions:

1) At high temperatures (T > 1880 K), at approximately what pressure is the transition to a simple three-phase assemblage of ferromagnesian silicate perovskite + magnesiowüstite + calcium silicate perovskite complete?

2) At lower temperatures (800 K < T < 1880 K), what is the stable phase assemblage at these same pressures?

3) Use "werami" to generate a 2-D grid of density values across your P-T space, using a grid density of 100x100 points. Then use "pstable" to plot a contour diagram of density from the resulting table file (probably named something like "example5_1.tab"), using a contour interval of 100 kg/m^3. Which reaction gives rise to the most rapid change in density in the entire P-T space? (The simplest way to do this may involve overlaying your density-contour plot on top of your phase-diagram plot and stabbing your pencil through the paper at the point(s) of maximum density gradient...)