SIO 224 Homework 4

1) Composition of the lower mantle

The code to do this is on the website and is in a tar file of eos.dir (eos.dir.tar)

As you have heard in class, the lower mantle between pressures of 30GPa and 120Gpa is believed to be relatively homogeneous and of fairly simple mineralogy. Above this pressure, upper mantle minerals are still transforming to their high pressure counterparts, and, at higher pressures, new phase transformations are now thought to be possible.

Therefore, between 30GPa and 120GPa, we think we can use 1D seismic models of the Earth in concert with equilibrium thermodynamics to determine the bulk composition of the mantle (later in the class, we shall discuss other types of transitions such as spin transitions which may violate these conditions).

Below about 800km depth, we believe that only 3 mineral species may be abundant: magnesiowustite (or ferropericlase) $(Mg,Fe)O$; magnesium-iron silicate perovskite $(Mg,Fe)SiO_3$; and smaller amounts of calcium silicate perovskite$CaSiO_3$. Aluminum is probably accommodated in the magnesium-iron silicate perovskite but its effect on seismic velocities is currently controversial (and possibly negligible). This means that a small number of parameters can be used to describe the composition of the lower mantle:

- X_{Pv} – the mole fraction of magnesium-iron silicate perovskite
- X_{Ca} – the mole fraction of calcium silicate perovskite
- X_{Mw} – the mole fraction of magnesiowustite. This doesn't have to be specified since $X_{Mw} = 1. - X_{Pv} - X_{Ca}$
- X_{Fe} – the fraction of Mg/Fe sites occupied by Fe: Fe/(Mg+Fe) which, from geochemical constraints, is close to 0.1.
- K_D – the partition coefficient which describes the partitioning of iron between magnesiowustite and magnesium-iron silicate perovskite. This is defined as

$$K_D = \frac{X_{Pv}^{Fe}/X_{Pv}^{Mg}}{X_{Mw}^{Fe}/X_{Mw}^{Mg}}$$

The value of this parameter is not very certain. Some experiments indicate that most of the iron goes into magnesiowustite with $K_D \simeq 0.25$ but other experiments, in the presence of aluminum, indicate that iron goes equally into both phases implying $K_D \simeq 1$. Equilibrium thermodynamics indicates a K_D of about 0.8. Fortunately, this parameter does not seem to have much effect on the properties of the resulting phase assemblage though you are encouraged to play with it.

The final parameter we need to specify to calculate the seismological properties of a particular mineral assemblage is the temperature. In the code you are given, we assume that the temperature profile is adiabatic and this is specified by the temperature at the 660km discontinuity (thought to be about 1900K though, in certain circumstances, could be larger). The code extrapolates this through the lower mantle using the thermal properties of magnesium-iron silicate perovskite which is the dominant mineral in the lower mantle. The resulting temperature profile is rather insensitive to the thermal properties assumed (except for the boundary condition on temperature at the 660).

Thus, the following five numbers specify a mantle composition and temperature:

$$X_{Fe}, K_D, X_{Pv}, X_{Ca}, T_{660}$$

For a pyrolite composition, $X_{Pv} \simeq 0.62, X_{Ca} \simeq 0.05, X_{Fe} \simeq 0.10$. K_D is probably between 0.25 and 1. For a composition closer to a chondritic meteorite, X_{Pv} is larger, on the order of 0.75, at the expense of X_{Mw}.

Program eos_mu2 allows you to experiment with these numbers to see what composition/temperature combinations can fit the lower mantle of PREM. We use the density, bulk sound speed, and the shear velocity to do this comparison. We use the Mie-Gruneisen equation of state to specify the properties of each candidate mineral: $MgO, FeO, MgSiO_3, FeSiO_3, CaSiO_3$. The properties of each mineral at a particular, P,T state are computed then averaged according to their molar fractions and iron partitioning to get the final

properties of the assemblage. These are then compared with PREM at a discrete number of pressures and a couple of measures of misfit for each parameter are returned: χ^2/N and the maximum deviation in terms of standard deviations. (Given our discussion of resolving power of 1D models, we take the uncertainty in density to be 0.5% and the uncertainty in seismic velocities to be 0.1%). The mineralogical data on shear velocity is sparse and so comparisons with V_s are less reliable than comparisons with density and V_c – however, it turns out that V_s is critical for illiminating some compositions.

Recently, the code has been changed to add a Q correction to account for the fact that the seismic parameters are measured at 1Hz or less while the lab parameters are measured at GHz to MHz. This correction follows the procedure in Matas et al, 2007 but is not too important for the lower mantle.

You should start by specifying X_{Pv} for a trial starting composition (e.g. somewhere between 0.62 and 0.68 for pyrolite). Here are some typical behaviors which may help you get a good answer:

- Increasing temperature reduces both velocities and density but reduces V_s the most.
- Increasing X_{Fe} increases density and reduces V_s but has little effect on V_c
- Increasing X_{Ca} increases V_s but has little effect on density or V_c
- Changing K_D has a relatively small effect so this can be fixed initially

Remember that you cannot keep increasing X_{Pv} and X_{Ca} without limit – their total should be less than or equal to 1. If it is 1 then you have eliminated magnesiowustite from the lower mantle.

Choose three values for X_{Pv} covering an extreme range of lower mantle compositions. I suggest the values 0.64, 0.74, 0.84 (corresponding to "pyrolite", "chondritic", and "solar"). Find the best values for the other parameters described above to fit PREM.

1) Are any compositions disallowed?

2) If you only know density and bulk sound speed, are any compositions disallowed?

3) What are the implications of the temperatures at 660km depth that you need to fit PREM. Does this lead you to a preferred model?

4) Did you have to do outrageous things to X_{Fe} and X_{Ca} to fit PREM?

5) The predictions of the code are rather sensitive to a few of the EOS elastic parameters – particularly the pressure derivatives of the bulk and shear modulus for magnesium-iron silicate perovskite (the dominant mineral in the lower mantle) as these change the shape of the velocity profiles of V_c and V_s. Feel free to change the parameters in subroutine assemb to investigate this. Currently, K_0' is set to 3.9 or so (what did you get from the previous homework problem?) but changing this to 4.1 (the Stixrude preferred value) can make quite a difference. The recent Murakami et al paper also suggests that G_0' should be 1.56 rather than the 1.7 used in the code. This also has some interesting effects.

Some notes on the code: you need the program eos_mu2.f which is written in good old F77. You also need the file prmtab2 which should be in the same directory as eos_mu2. This file is an ascii table of the properties of PREM interpolated to some particular pressures.

The code asks for the parameters described above which specify the composition and temperature of your particular lower mantle. The code outputs the predictions of the model (to file fort.66) at 19 pressures between 30GPa and 120GPa for the seismic properties and density along with the deviations from PREM defined by

$$\frac{V - V_{PREM}}{\sigma}$$

where σ is taken as 0.5% for density and 0.1% for velocities. fort.67 consists of colums of ascii output where the columns are:

$$T, P, \rho^{PREM}, \rho, \rho^{dev}, V_c^{PREM}, V_c, V_c^{dev}, V_s^{PREM}, V_s, V_S^{dev}, erho, evc, evs$$

The last three columns are errors determined from the uncertainties in the mineral physics. The program actually does 100 calculations at each pressure using mineral physics parameters with noise added based on their experimental uncertainties. The mean and standard deviation of these 100 models is what is output.

The run file for the code "runeos2" also uses the program "plotxy" to make figures of the fits and deviations of the various parameters as a function of pressure. You can replace plotxy with your favorite plotting program if you want to though it is provided in the code package.

2) Phase transitions

You have a binary ideal mixture of two components (A and B) undergoing a phase transformation. Pure end member A transforms at 20GPa and pure end member B transforms at 18GPa. You may take the volume change of each end member transformation to be identical and you should choose $\Delta V/RT$ to be first 0.2 and then 1. For each case:

1) What is the partition coefficient

2) Plot the phase loop

3) For $X = 0.1, 0.5, 0.9$, calculate the pressure at which you enter and leave the phase loop and plot the "yield" of the high pressure phase as you cross the phase loop. Estimate the effective width of the phase transformation.