

Padova Day 3

Any files, programs, etc. referenced in the script below can be copied from:

www.perplex.ethz.ch/perplex/tutorial/padova_phase_diagram_section_workshop_2023/padova_day_3.zip

Exercise 1. Modify the P-T phase diagram section input file you made on Day 2. To make an isobaric ($P = 4$ GPa) T-X phase diagram section that shows the influence of the volatile components (H_2O , CO_2) on phase relations. To do this you need only edit the thermodynamic component section of the input to read, the compositional variable will describe the variation between the 1st and 2nd bulk compositions:

```
begin thermodynamic component list
Na2O  2  0.328000      0.328000      0.000000      molar amount
MgO   2  1.623000      1.623000      0.000000      molar amount
Al2O3 2  1.497000      1.497000      0.000000      molar amount
K2O   2  0.580000E-01   1.497000      0.000000      molar amount
CaO   2  2.258000      2.258000      0.000000      molar amount
TiO2  2  0.138000      0.138000      0.000000      molar amount
FeO   2  1.370000      1.370000      0.000000      molar amount
SiO2  2  7.490000      7.490000      0.000000      molar amount
H2    2  0                1.460000      0.000000      molar amount
C     2  0                0.659000      0.000000      molar amount
O2    2  0                1.389         0.000000      molar amount
end thermodynamic component list
```

Exercise 2. This exercise will replicate (or refine) various calculations from Connolly & Galvez 2018 (https://www.perplex.ethz.ch/papers/connolly_eps1_2018.pdf) relevant to the release of devolatilization-generated fluids during subduction of oceanic sediment. Use BUILD to make an input file with the following parameters:

- Thermodynamic data file: DEW19HP622ver.dat
- Option file: perplex_option.dat [default]
- Computational mode: 5 [1d Phase fractionation]
- Thermodynamic components: [list can be pasted into BUILD]

H2
C
Si
Al
Fe
Mg
Ca
Na
K
O2
S2

- Enter path coordinates from file: subduction_PT_path.dat
- Molar amounts of the components: 0.405 0.068 0.975 0.234 0.073 0.062 0.106 0.078 0.044

1.567 0.01

- Excluded phases: f3clin, naph, nta and the list in padova_excluded_species.txt
- Solution models:

COH-Fluid
Omph(GHP)
Mica(CF)
Do(HP)
M(HP)
Grt(JH)
Chl(HP)
feldspar
Stlp
Pu

- Run the calculation in VERTEX without fractionating any phases (i.e., a closed system model). Run PSSECT to plot the result, sample the results by running WERAMI in mode 1 at node 600. Copy the result into a text file so you can compare it to later results (or use MEEMUM to create the same output by requesting a print file). Although the input composition is given in terms of elemental components it corresponds to a composition consisting entirely of reduced oxides (FeO, H₂O, CO₂, FeS, etc), why then does graphite appear as a stable phase?
- Use WERAMI in mode 3, property choice 40 to extract the simple back-calculated chemistry of the fluid along the subduction path. Using `perple_x_plot` (MATLAB), `PSTABLE`, or `PyWERAMI` to visualize the data. Compare this to the true composition of the fluid obtained using property choice 36 (for the fluid). You can also plot P and T as a function of node # to visualize the P-T path.
- Because `aq_output` is set to T (default), WERAMI automatically outputs simple back-calculated fluid speciation. Edit the option file to set `aq_lagged_speciation` to T and repeat the calculation. Compare the fluid composition and phase proportions. Does lagged speciation increase or decrease the stability of the fluid? Is the simple back-calculated speciation obtained in part A comparable the lagged (i.e., “optimized”) fluid composition?
- Reset `aq_lagged_speciation` to F (or default)
- Make a copy of the input file generated in Part A with a new name so that you don’t overwrite your previous results. Run VERTEX again, but this time fractionate the fluid phase (COH-Fluid).
- Use WERAMI in mode 3, property choice 25, to plot the mineral modes (either normal or cumulative, or both). If you use cumulative modes, setting the option `fancy_cumulative_modes` to T, generally improves legibility. Use WERAMI in mode 1 (or look at the *.tab file) to satisfy yourself that you can identify/label the phase fields.
- Set `aq_lagged_speciation` to T. Repeat steps E & F with lagged speciation. Compare the mineral proportions with and without lagged speciation. If you are using MATLAB, then you can edit the `perple_x_plot` script (change linestyle from ‘-’ to ‘--’ and easily superimpose the results. If you are using `PSTABLE` the results can be superimposed using Illustrator, CoreDraw, etc.
- Using the output created in Part G, run WERAMI in mode 3, property choice 40 to extract the fluid chemistry. Plot the bulk chemistry of the fractionated fluid and compare the result to that

obtained by simple back calculation in part B. The molecular solvent speciation (COH species) and electrolyte speciation may also be of interest.

- I) The compositions obtained in part H and G are relative. For mass balance calculation absolute quantities are required. To obtain these set the “absolute” option to T, additionally to see the cumulative mass loss set “cumulative” to T and run WERAMI in mode 3 for property choice 36 (fluid only). Plot the result and try to rationalize the result in terms of mineralogical variations. N.B.: the cumulative and absolute options only function correctly for property choice 36 and will result in nonsensical output for property choice 40. Additionally, property choice 36 labels for component amounts indicate the units specified by the composition_system option (default mass) but units actually used for phase are those specified by composition_phase (default molar). The reason for this oddity is that by default option 36 outputs both phase and system quantities and only one label is generated for each property.