

Perplex Tutorial I: Installation and a simple ternary diagram

Basics

Perplex is a collection of programs, each designed to accomplish a different task. These are command-line programs, and have been compiled for Windows, Mac OS X, and Linux. The best way (on Windows and OS X) to run the programs is to make a new task folder for each problem you wish to solve.

Installation: Mac

Important: for this stuff to work, you have to follow the directions exactly. Don't change capitalization, spelling, spaces, punctuation, or anything else. Be sure to put everything exactly where instructed.

First, get and install TEXTWRANGLER; it's free. You'll need it. Be sure to run it once and install the command-line tools as well (a checkbox on the registration window).

<http://www.barebones.com/products/textwrangler/download.html>

Also download Dave's Perplex Helpers from the class website. Unzip it if necessary, and leave it in your Downloads folder for now.

Download the current Perplex programs from the Perplex website: **http://www.perplex.ethz.ch/perplex/ibm_and_mac_archives/OSX/**

If you're not sure which version is the best, choose any of the latest-numbered ones. More recent ones are likely better. Unzip it if necessary after it's downloaded. Rename the folder to "Perplex" and move or copy it to your Applications folder. The files should be a set of things starting with "actcor" and "build".

Download the current Perplex data files: **http://www.perplex.ethz.ch/perplex/ibm_and_mac_archives/**

(look for a file with "data files" in the name). These should be a set of files ending in ".dat". Unzip the file if necessary, and rename the folder to "datafiles". Move the folder into the Perplex folder that should now be inside your Applications folder, so it lives at /Applications/Perplex/datafiles.

Because Perplex development happens on a Windows system, the data files all have Windows-type line endings. (Windows and OS X/Linux use different conventions for what character(s) signal the end of a line in a text file). You need to convert the line endings to OS X type.

I've provided a little program called MAKEOSXLINEENDINGS in the Dave's Perplex Helpers folder. Drag the datafiles folder onto this, and follow the prompts to convert all the files ending in ".dat".

The last step required is to make the programs accessible from anywhere in the file system, not just in the local database. To do this, you need to edit an invisible file that contains settings used in the command-line environment. Open Terminal and type this (exactly):

```
edit ~/.bash_profile
```

TextWrangler should open a file, which may or may not be blank. From TextWrangler, open the file called "Bash Profile Stuff.txt" that is supplied in Dave's Perplex Helpers, and copy its contents into the .bash_profile file. Save.

This next step is not required, but might make things nicer for you. I'm not a big fan of the default Terminal settings. I've supplied a settings file (in Dave's Perplex Helpers) that you can import into Terminal. Just double-click the file, and you will get a new settings choice that you can make the default style if you wish, by going to Terminal's Preferences and finding the new settings in the list.

This next is also not required, but will make life a lot easier, I expect, by making a quick-access file listing command that is easier to read than the default style. Type this in Terminal:

```
edit ~/.bashrc
```

TextWrangler should open a file, which may or may not be blank. From TextWrangler, open the file called "Bash RC Stuff.txt" that is supplied in Dave's Perplex Helpers, and copy its contents into the .bashrc file. Save.

The last thing you need to do is to move or copy the programs OPEN TERMINAL WINDOW HERE and MAKE PERPLEX FOLDER from Dave's Perplex Helpers into the main Perplex Folder (in /Applications/Perplex). Be sure to also make an alias to MAKE PERPLEX FOLDER someplace accessible, or drag it into the Dock.

You are now installed. Quit Terminal (to be sure your changes are active for the rest of the Tutorial).

Installation: Windows

Important: for this stuff to work, you have to follow the directions exactly. Don't change capitalization, spelling, spaces, punctuation, or anything else. Be sure to put everything exactly where instructed.

First, get and install NOTEPAD++; it's free. It's way better than the built-in Notepad.

<http://notepad-plus-plus.org/download/v6.5.1.html>

Also download Dave's Perplex Helpers from the class website. Unzip it if necessary, and leave it in your Downloads folder for now.

Note: never just double-click a zipped archive to see/access its contents; this can cause tricky problems. Always extract the files by right-clicking the zip file and choosing Extract All. The freeware program 7ZIP (<http://www.7-zip.org/>) can make this, and other zip-related things, easier .

Download the current Perplex programs from the Perplex website: **http://www.perplex.ethz.ch/perplex/ibm_and_mac_archives/WINDOWS/**

If you're not sure which version is the best, choose any of the latest-numbered ones. More recent ones are likely better. If you are unsure whether your computer is 32- or 64-bit, choose 32.

Create a new folder in C:\Program Files (x86) called "Perplex". Extract the downloaded zip to this new folder (C:\Program Files (x86)\Perplex\). The files should be a set of things starting with "ACTCOR" and "BUILD". (Note: you will need Administrative access to do this. If you don't have that, then you should be able to put the programs anywhere, and modify these instructions accordingly.) (Note2: If you have a really old PC, then you won't have any folder called C:\Program Files (x86), only one called C:\Program Files. Use that instead.)

Download the current Perplex data files: **http://www.perplex.ethz.ch/perplex/ibm_and_mac_archives/** (look for a file with "data files" in the name)

Create a new folder called "datafiles" inside C:\Program Files (x86)\Perplex\. Extract the downloaded zip to this new folder (C:\Program Files (x86)\Perplex\datafiles\). These should be a set of files ending in ".dat".

The last thing you need to do in this part is to move or copy the programs `OPENCOMMANDWINDOWHERE.VBS` and `MAKEPERPLEXFOLDER.VBS` from Dave's Perplex Helpers into the main Perplex Folder (in `C:\Program Files (x86)\Perplex\`). Be sure to also make a shortcut to `MAKEPERPLEXFOLDER.VBS` someplace accessible (Desktop?), or drag it into the Start Menu to pin it there.

Check to make sure you did it right: inside `C:\Program Files (x86)`, there should be a folder called "Perplex". Inside that there should be a bunch of programs (starting with `ACTCOR` and `BUILD`), the two scripts `OPENCOMMANDWINDOWHERE.VBS` and `MAKEPERPLEXFOLDER.VBS`, and a folder called "datafiles". Inside the datafiles folder there should be a bunch of files including `hp02ver.dat`. In addition, there should be a shortcut to `MAKEPERPLEXFOLDER.VBS` pinned to the Start menu or on the Desktop or some other accessible place.

In addition, you will need some way to view and print PostScript files. The best is Adobe Illustrator, which allows you to edit the files as well. Next best is GhostScript/Inkscape (both free), which together allow you to view and edit PostScript files, and convert them to PDFs or EPS files. It can be obtained here:

<http://www.ghostscript.com/download/gsdnld.html>

After it has installed, check to see what version was installed, and whether it installed itself in `C:\Program Files`, or `C:\Program Files (x86)`. Do this by looking inside both Program Files folders for something called "gs". Look inside there for another folder that looks like "gs9.10". That is the version number (9.10 in this example).

Finally you need to be sure that the Perplex and ghostscript programs are accessible from wherever you are in the file system. To do that, you need to set or alter the PATH environment variable. To do this, right-click on Computer, then go to Properties, then Advanced, then Environment Variables, then select the PATH item in the lower box and click Edit. (If no PATH item is there, then create one.) In the PATH value (not the name), put this on the end:

```
;C:\Program Files (x86)\Perplex\;C:\Program Files (x86)\gs\gs9.10\bin\;C:\Program Files (x86)\gs\gs9.10\lib\
```

Be careful about capitalization colons vs. semicolons, spaces, etc. If you make an error, it won't work. You only need the initial semicolon if there was text there already. Semicolons separate entries in the PATH variable. Note that the text I provided assumes that ghostscript installed itself into `C:\Program Files (x86)`, and that the version of ghostscript that was installed was version 9.10. You'll need to adapt the command in case those things are not true for you.

To confirm you did this right, find and run a copy of `OPENCOMMANDWINDOWHERE.VBS` and in the window that appears, type `build`. If you don't see an error of the type "build is not a recognized program", then hit [Control]-C to break out, and try typing `ps2pdf`. If that also works, then try it with `gs`. If any of those failed, then you made an error with the PATH. Read this section again and try to fix whatever you messed up.

Ghostscript is good for viewing and converting files, but you also will want to anontate files. For that you can use Inkscape. You can get it here:

<http://inkscape.org/en/download/>

Download and install it, and if you had Ghostscript correctly installed, then Inkscape should be able to import postscript files for editing. It can save to PNG, which MS Word can import (for putting graphs into your final document(s)). You can also use the `PS2EPSI` program in ghostscript to turn the postscript output into something MS Word can import.

How to run Perplex

There is a script in Dave's Perplex Helpers called MAKE PERPLEX FOLDER which will take an existing (presumably empty) folder, copy the important data and options files to it, and open the folder in the Finder (OS X) or Windows Explorer (Windows). In the folder that gets produced, there is a script called OPENCOMMANDWINDOWHERE (Windows) or OPEN TERMINAL WINDOW HERE (OS X). You should use these scripts to run the programs, until you become more proficient. Note that if you run the Perplex programs from the primary folder (where the programs live) then you will end up with a very cluttered folder and it will be hard to keep track of things.

General comments

Here are some useful commands for those unfamiliar with the command-line:

| Task | Windows | OS X |
|---------------------------------|----------------------|---|
| List current directory path | <code>cd</code> | <code>pwd</code> |
| List files in current directory | <code>dir</code> | <code>ls</code> (or <code>l</code> ("ell") if you've installed the Bash RC Stuff) |
| Change directory to <i>foo</i> | <code>cd foo</code> | <code>cd foo</code> |
| Go "up" one directory level | <code>cd ..</code> | <code>cd ..</code> |
| Remove file <i>bar</i> | <code>del bar</code> | <code>rm bar</code> |

One useful trick on OS X: if you drag a file or folder into a Terminal window, the full path of that item will be printed at the current text prompt. So if you want to change the current directory to a folder, you can type "`cd` " (note the trailing space), and then drag the folder in, then hit return in Terminal to go there.

Programs in Perplex

This tutorial is based on the version of Perplex and datafiles available on November 15, 2013. In particular, these are based on Perplex 6.6.8. The programs you will use are:

- **BUILD** - this makes the datafile that tells VERTEX how to setup the calculation. You will spend most of your effort on BUILD.
- **VERTEX** - this does the calculation and saves the results.
- **PSVDRAW** - this takes the plotfile output from VERTEX and makes a PostScript plot from it. You can specify options to highlight particular aspects of the file.
- **PSSECT** - this operates much like PSVDRAW, but plots pseudosections, not phase diagrams
- **PSTABLE** - plots contours of properties from WERAMI output files.
- **WERAMI** - can make files to input into PSTABLE, but can also be used interactively to find out properties of the system at user-specified conditions.
- **MEEMUM** - calculates stable assemblage at particular P-T-X conditions.

There are others, but you should not need to use them for these tutorials, and perhaps not at all until you are much farther along in Perplex. The above list are the executable programs, but these need other files, including options files and thermodynamic data files as input, listed below.

- *hp02ver.dat* - This is the thermodynamic database of Holland and Powell (2002). You could run Perplex with other databases instead if you wished.
- *solution_model.dat* - This is the file with all the possible solution models that relate free energy of a phase to its composition. Note that many phases have multiple possible solution models that you might choose. Read the file for some guidance as to which is best for your problem.
- *perplex_option.dat* - Text file that sets certain calculation options
- *perplex_plot_option.dat* - Text file that sets certain graphical output options

Task 1 - Making a ternary phase diagram

This is one of the simplest tasks in Perplex. We will make a simple ternary phase diagram without any solid solution phases, and we will show how it changes with a change in conditions.

(Note: If you merely type stuff in by following this guide, you won't learn anything. You are expected to read all the prompts and ask questions if there are some that you don't understand. In later tasks you will be expected to redo this, changing your responses in various ways to achieve other results. If you don't actually read these, then you will be confused later.)

Building the run file

First run MAKE PERPLEX FOLDER. It will ask you to find a folder into which it will copy the needed input files. You should navigate to someplace convenient (like the Desktop or your Documents folder) and click the Create New Folder button. Call this new folder `task1`, (and on Windows, be sure it is selected before choosing it by clicking off then on it). Select the task1 folder you created and click OK or Choose to copy all the relevant files to this folder. Then open a command window in the task1 folder you made.

Run BUILD:

`build` (This is the font I will use for things you should type)

NO is the default (<cr>) answer to all Y/N prompts (This is the font I will use for text the program will print out)

```
Enter a name for this project (the name will be used as the
root for all output file names) [default = my_project]:
task1
```

```
Enter thermodynamic data file name, [default = hp02ver.dat]:
```

(Note that you can just hit return to accept any default option, and that NO is the default for all "Y/N" choices). Hit return here.

```
Enter the computational option file name, [default = perplex_option.dat]:
See: www.perplex.ethz.ch/perplex\_options.html
```

Hit return here.

```
The current data base components are:
```

```
NA2O  MGO  AL2O3  SIO2  K2O   CAO   TIO2  MNO   FEO   NIO   ZRO2  CL2
O2    H2O   CO2
```

```
Transform them (Y/N)?
```

N

```
Calculations with a saturated FLUID (Y/N)?
```

N

```
Calculations with saturated components (Y/N)?
```

N

```
Use chemical potentials, activities or fugacities as independent
variables (Y/N)?
```

N

```
Select thermodynamic components from the set:
```

```
NA2O  MGO  AL2O3  SIO2  K2O   CAO   TIO2  MNO   FEO   NIO   ZRO2  CL2
O2    H2O   CO2
```

Enter names, 1 per line, press <enter> to finish:

AL2O3

MGO

SIO2

[then hit enter. (do not type this text in)]

Specify computational mode:

- 1 - Unconstrained minimization
- 2 - Constrained minimization on a 2d grid [default]
- 3 - Constrained minimization on a 1d grid
- 4 - Output pseudocompound data
- 5 - Phase fractionation calculations

Use unconstrained minimization for Schreinemakers projections or phase diagrams with > 2 independent variables. Use constrained minimization for phase diagrams or phase diagram sections with < 3 independent variables.

1

The data base has P(bar) and T(K) as default independent potentials. Make one dependent on the other, e.g., as along a geothermal gradient (y/n)?

N

Specify number of independent potential variables:

- 0 - Composition diagram [default]
- 1 - Mixed-variable diagram
- 2 - Sections and Schreinemakers-type diagrams

0

Output a print file (Y/N)?

Y

Summary of valid make definitions:

| | MGO | AL2O3 | SIO2 |
|-------|------|-------|------|
| sil8L | 0.00 | 1.60 | 1.60 |
| fo8L | 4.00 | 0.00 | 2.00 |
| q8L | 0.00 | 0.00 | 4.00 |

Exclude pure and/or endmember phases (Y/N)?

N

Excluding phases makes the calculations speedier. In general, you should start by not excluding any phases, and if you get some weird phases forming, then exclude those, but only if you have a good reason. Only after you know what phases to consider might you exclude the others.

Include solution phases (Y/N)?

N

Enter calculation title:

Task 1

Specify values for:

P(bar) T(K)

For calculation 1, enter zeros to finish.

13000 1143

Specify values for:

P(bar) T(K)

For calculation 2, enter zeros to finish.

13000 1153

Specify values for:

P(bar) T(K)

For calculation 3, enter zeros to finish.

13000 1163

Specify values for:

P(bar) T(K)

For calculation 4, enter zeros to finish.

0 0

Now you are done with BUILD. Let's take a look at the file you made. Open the task1.dat file in either TextWrangler (OS X) or Notepad++ (Windows) and peruse the document. There is nothing magical about this file. BUILD has just made a text file. If you want to edit the file to see what parts control which behavior, or to make a similar run with slight changes, you can just make changes.

Doing the calculations

Run VERTEX to actually do the calculations:

vertex

Enter the project name (the name assigned in BUILD) [default = my_project]:

task1

```
Reading problem definition from file: task1.dat
Reading thermodynamic data from file: hp02ver.dat
Reading solution models from file: not requested
Writing print output to file: task1.prn
Writing plot output to file: task1.plt
```

```
Reading computational options from: perplex_option.dat
Writing computational option summary to file: not requested
```

Perple_X computational option settings for VERTEX:

| Keyword: | Value: | Permitted values [default]: |
|----------|--------|-----------------------------|
|----------|--------|-----------------------------|

Auto-refine options:

| | | |
|-----------------------|-----|-------------------|
| auto_refine | aut | off manual [auto] |
| auto_refine_factor_II | 6.0 | >=1 [10] |

Solution subdivision options:

| | | |
|----------------------|--------|------------------------|
| initial_resolution | 0.067 | 0->1 [0.067], 0 => off |
| stretch_factor | 0.016 | >0 [0.0164] |
| subdivision_override | off | [off] lin str |
| hard_limits | off | [off] on |
| pc_perturbation | 0.0050 | [5d-3] |

Thermodynamic options:

| | | |
|----------------------|---------|--|
| solvus_tolerance | aut | [aut] or 0->1; aut = automatic, 0 => p=c pseudo-compounds, 1 => homogenize |
| speciation_tolerance | 0.2E-04 | 0->1 [1e-3]; order-disorder speciation precision |
| T_stop (K) | 0.0 | [0] |

```

T_melt (K)           873.0      [873]
order_check         on         off [on]
approx_alpha        T          [T] F
Anderson-Gruneisen  F          [T] F
site_check          F          [T] F
speciation_max_it   20        [40]

```

Input/Output options:

```

dependent_potentials on         off [on]

```

Information file output options:

```

option_list_files   F          [F] T; echo computational options
pseudocompound_file F          [F] T; echo static pseudocompound compositions
auto_refine_file    F          [F] T; echo auto-refine compositions

```

Worst case (Cartesian) compositional resolution (mol):

```

Exploratory stage:  0.372E-02
Auto-refine stage:  0.207E-03

```

Adaptive minimization will be done with:

```

3 iterations in the exploratory stage
4 iterations in the auto-refine stage

```

To change these options see: www.perplex.ethz.ch/perplex_options.html

Summary of valid make definitions:

| | MGO | AL2O3 | SiO2 |
|-------|------|-------|------|
| sil8L | 0.00 | 1.60 | 1.60 |
| fo8L | 4.00 | 0.00 | 2.00 |
| q8L | 0.00 | 0.00 | 4.00 |

** Starting auto_refine computational stage **

```

Computing the compositional phase relations at condition 1
cycle      1      1      1
cycle      2      2      3
cycle      3      4      6
cycle      4      7      7
Computing the compositional phase relations at condition 2
cycle      1      1      1
cycle      2      2      3
cycle      3      4      6
cycle      4      7      7
Computing the compositional phase relations at condition 3
cycle      1      1      1
cycle      2      2      3
cycle      3      4      6
cycle      4      7      8
cycle      5      9      9

```

Viewing the results

Good! Now you have completed the calculations. You can see the text output in the print (.prn) file by opening task1.prn in a text editor. Note that it shows the stable assemblage at each set of conditions. In order to get a diagram of the results, you can make a graphics file from the plot (.plt) file (the plot file is also just a text file, but doesn't make much sense to a human reader, so we don't typically examine it ourselves.):

psvdraw

Enter the project or plot file name [i.e., without the .plt suffix]:

task1

Perple_X plot options are currently set as:

| Keyword: | Value: | Permitted values [default]: |
|--------------------------|-----------|-----------------------------------|
| axis_label_scale | 1.20 | [1.2] (rel) |
| bounding_box : | | |
| | 0 | [0] x-min (pts) |
| | 0 | [0] y-min (pts) |
| | 800 | [800] x-length (pts) |
| | 800 | [800] y-length (pts) |
| field_fill | T | [T] F |
| field_label | T | [T] F |
| field_label_scale | 0.75 | [0.72] (rel) |
| font | Helvetica | |
| grid | F | [F] T |
| half_ticks | T | [T] F |
| line_width | 1.00 | 0-99 [1.] (pts) |
| picture_transformation : | | |
| | 0.180 | [0.18] x-scale (rel) |
| | 0.180 | [0.18] y-scale (rel) |
| | 130. | [0.18] x-translation (pts) |
| | 220. | [0.18] y-translation (pts) |
| | 0.00 | [0.0] rotation (deg) |
| plot_aspect_ratio | 1.000 | [1.0] x_axis_length/y_axis_length |
| replicate_label | 0.250 | 0->1 [0.025] |
| splines | T | [T] F |
| tenth_ticks | F | [F] T |
| text_scale | 1.000 | [1.] (rel) |

To change these options edit or create the plot option file

See: www.perplex.ethz.ch/perplex_plot_options.html

PostScript will be written to file: task1.ps

Modify the default plot (y/n)?

N

Now the results are saved in a file called `task1.ps`. This is a postscript file. You can view and edit it in Acrobat Illustrator (or a wealth of other programs). You can view it on the Mac in the built-in Preview application (just double-click it). On Windows, if you don't have Illustrator, you will need to use GhostScript or some other program. If you followed the Windows installation instructions, you should be able to open the `task1.ps` file in either Ghostscript or Inkscape.

When you view the file, you should see the image at right (note that `spr4` stands for sapphirine; all abbreviations can be found in the `hp02ver.dat` file).

Answer these questions:

Question I-1: What are the reactions shown here by the changes among the diagrams?

Question I-2: Can you find all of them on the P-T diagram below?

Question I-3: Are they at the correct P-T conditions?

Let's exclude sapphirine. In a text editor, go back and make a copy of your `task1.dat` file; call it `task1a.dat`. In that new file, between the lines:

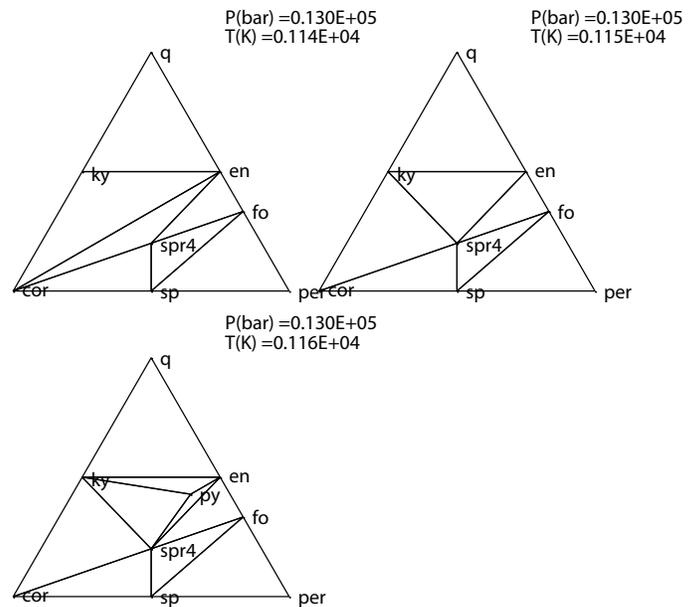
```
begin excluded phase list
end excluded phase list
```

type "`spr4`" and "`spr7`" (these are two varieties of sapphirine; put each on its own line). Change the calculation title to "`Task1a`" on line 5. Save this file. Now re-run VERTEX and PSVDRAW. Be sure to answer that your project is now "`task1a`" not "`task1`".

Question I-4: Examine your output; how is it different? Does this make sense given your answer to question 1 above? Explain.

Question I-5: Finally, make a copy of the `task1.dat` file, and call it "`task1b`". Choose another reaction on the P-T diagram below (try not to duplicate the points chosen by your classmates) and calculate diagrams across that reaction as well, by replacing the P-T-X lines near the end of the `task1b.dat` file. Do not exclude sapphirine. Run VERTEX and PSVDRAW again. What reaction did you replicate?

Turn in the three plots (`task1`, `task1a`, `task1b`), along with the answers to questions I-1 through I-5. These should be in a single MSWord document, with the figures embedded. If you are unsure whether your figures are embedded, then try opening the document on somebody else's computer, or a fresh one in the computer lab.



P-T diagram for the $\text{Al}_2\text{O}_3\text{-MgO-SiO}_2$ system

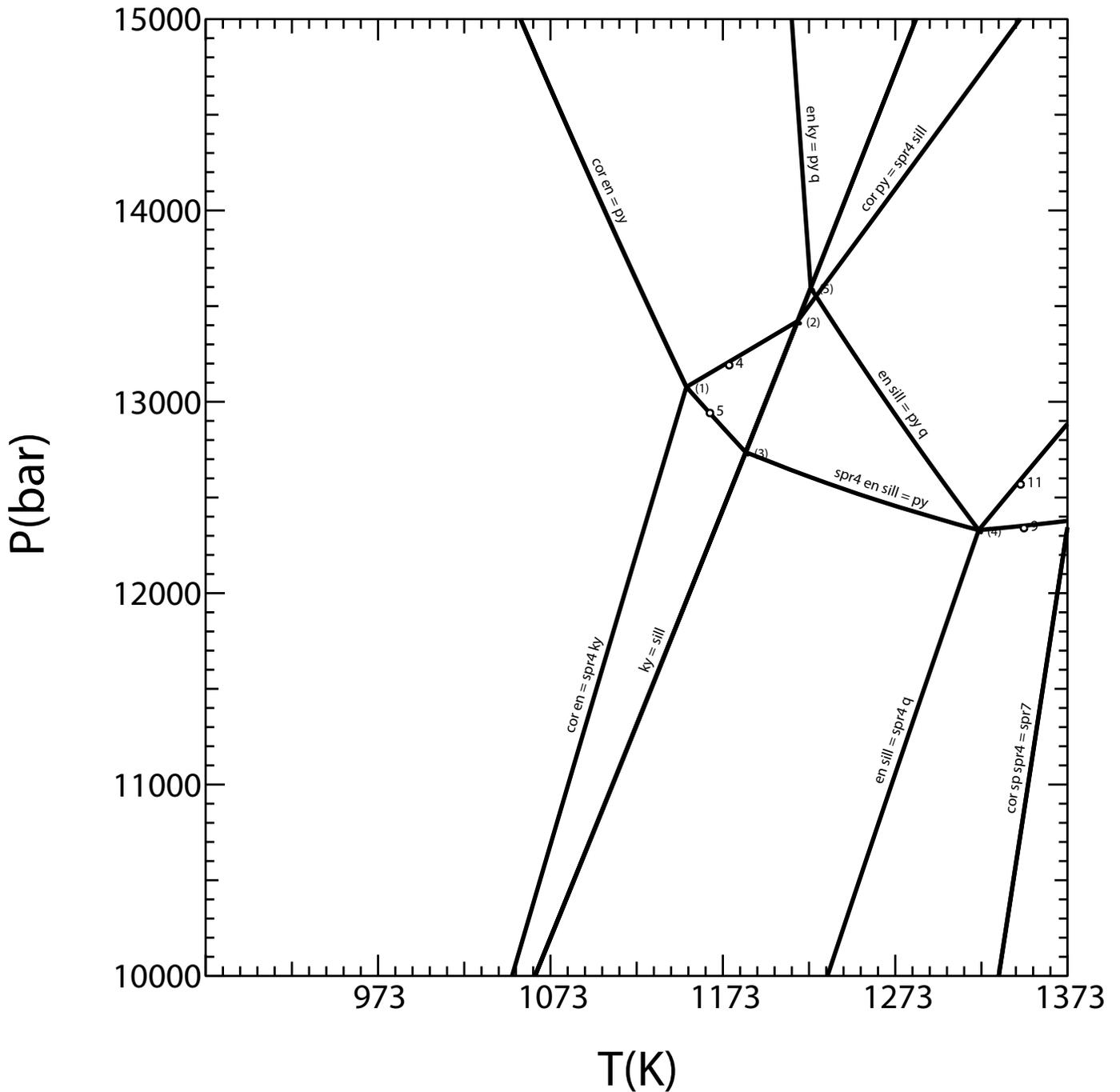
Reaction codes (phases on the right side of the “=” are on the high-T side of the reaction):

4: cor py = spr4 ky

5: spr4 en ky = py

9: py = spr4 en q

11: py sill = spr4 q



Perplex Tutorial II: P-T Diagrams

In contrast to the previous assignment, you will not be given detailed instructions, only guidance for those parts that were not covered in detail in Tutorial 1. In this assignment, you will use Perplex to create P-T diagrams. First you will make a simple diagram, then some more complex ones.

Task 2 - Re-creating the Aluminum Silicate Phase diagram

Perplex refers to P-T diagrams as Schreinemakers diagrams; making them can be a very simple task in Perplex. You may wish to refer to Task 1 for the prompts not covered here (give the same responses as before).

Building the run file

1. Choose a different folder and project name than last time, perhaps "task2"
2. For now, do not perform the calculations with either a saturated fluid phase or a saturated component.
3. When you choose oxide components, choose only Al_2O_3 and SiO_2 , since we're just looking for the stability of the Al_2SiO_5 minerals.
4. The computation mode should be unconstrained minimization.
5. For the number of independent potential variables, choose 2 (P & T).
6. Make temperature the x axis.
7. Perform the calculation from 250°C - 750°C, and from 1 kbar to 6 kbar (Note that Perplex wants temperature in Kelvins and pressure in bars). Note also that having the ranges be nicely divisible by 5 makes for nicer axes; here we have ranges of 500°C and 5 kbar.
8. Don't exclude any phases.
9. Don't include any solution phases, either.
10. After running BUILD, edit the perplex_option.dat file and make sure that `short_print` is set to `off`.

Results

Run VERTEX and PSVDRAW as usual to get the results. First, examine the print (.prn) file you made. Note that the only phases being considered are those containing only Si, O, and Al:

Phases and (projected) mol fraction SiO_2 :

| | | | | | | | |
|------|-------|-------|-------|------|-------|-----|-------|
| and | 0.500 | ky | 0.500 | sill | 0.500 | q | 1.000 |
| trd | 1.000 | crst | 1.000 | coe | 1.000 | stv | 1.000 |
| cor | 0.000 | silL | 0.500 | qL | 1.000 | qGL | 1.000 |
| coGL | 0.000 | sil8L | 0.500 | q8L | 1.000 | | |

Next the file tells you what is stable at the low-P, low-T corner of your calculation region. In this case, you could have either corundum + kyanite, or kyanite + quartz:

the stable assemblages at:

```
T(K)      = 523.000
P(bar)    = 1000.00
```

are (variance flag in parentheses):

```
cor      -ky      (0)   ky      -q      (0)
```

Question II-1: What determines whether a rock would actually have corundum + kyanite or kyanite + quartz at 250°C and 1 kbar?

Now, check out the P-T graph you made.

Question II-2: If kyanite is apparently stable at such low grades (250°C & 1 kbar), why do we think of kyanite as being a high-grade mineral?

Next in the print file, each reaction (i.e., line of equilibrium) is described as a set of P-T coordinates. The ΔS and $-\Delta V$ (note the negative!) values are the ΔS and $-\Delta V$ of reaction, to be used in the Clausius-Clapeyron equation.

Question II-3: What is the slope of the Ky-And reaction line (from the ΔS & $-\Delta V$ values)?

Finally, the coordinates of the invariant point (triple point) are given. Note that it is listed as "(1-0)".

Question II-4: How do the coordinates of the invariant point compare to the Holdaway & Mukhopadhyay (1993) value of 3.75 ± 0.25 kbar and 504 ± 20 °C? Why might they be different?

In addition to the coordinates of the invariant point, the phases stable at the point are listed. Corundum is included, because in general the composition of the rock in the SiO_2 - Al_2O_3 system will not be exactly Al_2SiO_5 . Why isn't it quartz along with the aluminum silicates? Try going into the build file ("task2.dat") and switching the AL_2O_3 and SiO_2 lines., and then run VERTEX again. When you view the new print file, you'll see that quartz is now listed along with the aluminum silicates.

Copy the hp04ver.dat dataset into the task2 folder, and make a modified copy ("task2a") of the build file that uses hp04ver.dat instead of hp02ver.dat. (You might have to download the datafiles from the Perplex website to get hp04ver.dat; be sure to change the line endings if necessary).

Question II-5: How does the diagram differ from the earlier one? How does the triple point compare to the Pattison (1992) value of 4.5 ± 0.5 kbar and 550 ± 35 °C?

Task 3 - Enhancing the Aluminum Silicate Phase diagram

The diagram you made in Task 2 is fine for most purposes, but in reality the stability of these minerals is limited by other reactions at low temperatures. We'll redo the above work, but make it more realistic by including a water-rich fluid phase and assume quartz is present. These are good assumptions for almost any rock likely to include enough aluminum to make an aluminum silicate.

Building the run file

1. Choose a different name than last time, perhaps "task3"

2. Switch back to the hp02ver.dat dataset.**3. This time, perform the calculations with a saturated H₂O-only fluid phase:**

Calculations with a saturated FLUID (Y/N)?

Y

Select the independent saturated FLUID components:

H2O CO2

Enter names, 1 per line, press <enter> to finish:

For C-O-H fluids it is only necessary to select volatile species present in the solids of interest. If the species listed here are H₂O and CO₂, then to constrain O₂ chemical potential to be consistent with C-O-H fluid speciation treat O₂ as a saturated component. Refer to the Perple_X Tutorial for details.

H2O**4. Also assume that quartz is present, and thus requires a saturated SiO₂ component:**

Calculations with saturated components (Y/N)?

Y

Select < 6 saturated components from the set:

NA2O MGO AL2O3 SiO2 K2O CAO TIO2 MNO FEO NIO ZRO2 CL2
O2 CO2

Enter names, 1 per line, press <enter> to finish:

SiO2**5. Then when you choose thermodynamic components, the only one you will need will be Al₂O₃.****6. You will need to enter fluid properties:**

Select fluid equation of state:

- 0 - X(CO2) Modified Redlich-Kwong (MRK/DeSantis/Holloway)
- 1 - X(CO2) Kerrick & Jacobs 1981 (HSMRK)
- 2 - X(CO2) Hybrid MRK/HSMRK
- 3 - X(CO2) Saxena & Fei 1987 pseudo-virial expansion
- 4 - Bottinga & Richet 1981 (CO2 RK)
- 5 - X(CO2) Holland & Powell 1991, 1998 (CORK)
- 6 - X(CO2) Hybrid Haar et al 1979/CORK (TRKMRK)
- 7 - f(O2/CO2)-f(S2) Graphite buffered COHS MRK fluid
- 8 - f(O2/CO2)-f(S2) Graphite buffered COHS hybrid-EoS fluid
- 10 - X(O) GCOH-fluid hybrid-EoS Connolly & Cesare 1993
- 11 - X(O) GCOH-fluid MRK Connolly & Cesare 1993
- 12 - X(O)-f(S2) GCOHS-fluid hybrid-EoS Connolly & Cesare 1993
- 13 - X(H2) H2-H2O hybrid-EoS
- 14 - X(CO2) Pitzer & Sterner 1994; Holland & Powell mixing 2003
- 15 - X(H2) low T H2-H2O hybrid-EoS
- 16 - X(O) H-O HSMRK/MRK hybrid-EoS
- 17 - X(O)-f(S2) H-O-S HSMRK/MRK hybrid-EoS
- 18 - X(CO2) Delany/HSMRK/MRK hybrid-EoS, for P > 10 kb
- 19 - X(O)-X(S) COHS hybrid-EoS Connolly & Cesare 1993
- 20 - X(O)-X(C) COHS hybrid-EoS Connolly & Cesare 1993
- 21 - X(CO2) Halbach & Chatterjee 1982, P > 10 kb, hybrid-EoS
- 22 - X(CO2) DHCORK, hybrid-EoS
- 23 - Toop-Samis Silicate Melt
- 24 - f(O2/CO2)-N/C Graphite saturated COHN MRK fluid
- 25 - H2O-CO2-NaCl Aranovich et al. 2010
- 26 - O-Si Silicate vapor RK EoS

5

There are lots of choices here; option 5 is a good one for many calculations, unless you have a good reason to choose another. There is guidance on these options in the Perplex documentation.

7. The program will ask you for the sectioning value for $Y(\text{CO}_2)$. Because you want a pure- H_2O phase, you should say zero.
8. Everything else should be as in tasks 1 and/or 2.

Results

Run VERTEX and PSVDRAW as usual to get the results. Examine the plot, and note the difference between this one and the previous one.

Question II-6: Looking at the set of minerals (you may wish to look up formulas), what is the key chemical difference in the system that allows pyrophyllite and kaolinite to form?

Question II-7: In the light of your new plot, do you have a different perspective on why we consider kyanite a high-grade mineral now?

Task 4 - Make your own

Now do the same thing, but plot a P-T diagram for some other simple chemical system. Choose whether to have a fluid or not, and whether quartz is present or not (and possibly other oxide phases), and choose one or two other oxides. If you like, you can try to replicate a diagram in Spear (1993) (but I would suggest staying away from systems with both Fe and Mg, and anything with Mn). See what you get.

Question II-8: Describe the setup you chose and what, if any, rock type your setup might apply to. Note particularly whether there are phases that are listed as multiple end-members, but are in reality solid solutions (e.g., diopside and hedenbergite).

Turn in your four P-T graphs (tasks 2, 2a, 3, & 4), and answers to question II-1 through II-8.

Perplex Tutorial III: Dealing with solid solutions

Task 5 - T-X_{MgO} diagram with solid solutions

Now for the first time we'll deal with solid solutions. Perplex deals with solid solutions by essentially creating a whole set of pseudocompounds (intermediate compositions), and treating each of them like a separate phase. Thus, if an olivine with composition Fo₈₀ has a lower free energy than Fo₈₅ at a particular P-T condition, then that Fo₈₀ olivine will be listed as the stable olivine.

We will plot the reactions that occur in the system K₂O-MgO-FeO-Al₂O₃-SiO₂-H₂O. However, to reduce the problem to one with only two thermodynamic components, water will be treated as a saturated phase, and we will project from SiO₂, Al₂O₃, and K₂O. This is a bit like projecting onto the AFM triangle, but requiring that all the assemblages will coexist with quartz, aluminum silicate, and muscovite or K-feldspar.

Building the run file

1. Choose a different name than last time, perhaps "task5"
2. As in task 3, perform the calculations with a saturated **H₂O-only** fluid phase, so list only H₂O in the "independent saturated phase components" list, and set Y(CO₂)=0.
3. Also assume that quartz, aluminum silicate, and muscovite/kspar are present, and thus require saturated SiO₂, Al₂O₃, and K₂O components (in that order).
4. When you choose thermodynamic components, the only ones that will be variable (and thus in the list) are FeO and MgO; in order for the plots to all come out the same, put FEO first, and MGO second.
5. Choose gridded optimization for the computation mode ("Constrained minimization on a 2d grid").
6. The x-axis variable should be the bulk composition ("Composition X(C1)* (user defined)").
7. Temperature should be the y-axis variable.
8. Plot the range of conditions: P=7 kbar, T= 500-650°C, and Y(CO₂)=0.0.
9. You do not want to constrain saturated components, nor specify component amounts by weight (we'll use molar proportions):

```
All thermodynamic components must be constrained,
constrain saturated components also (Y/N)?
```

N

```
Specify component amounts by weight (Y/N)?
```

N

10. You want the x-axis to range from FeO to MgO. The bulk composition formulation for this centers around the idea of a variation between two end-member bulk compositions (C0 and C1). C0 should be pure FeO and C1 should be pure MgO:

The bulk composition of the system will be computed as:

$$C = C0*(1-X(C1)) + C1*X(C1)$$

where X(C1) varies between 0 and 1, and C0 and C1 are the compositions

specified next.

To compute bulk compositions as: $C = C0 + C1 * X(C1)$
change the computational option keyword `closed_c_space`.

Enter molar amounts of the components:

FE0 MGO
to define the composition C0

1 0

Enter molar amounts of the components:

FE0 MGO
to define the composition C1

0 1

11. When BUILD asks if you want to exclude phases, you should say yes. It will ask if you want to be prompted for phases: you don't. Then enter only `a fchl`. This will speed up the calculation by limiting the range of chlorite compositions Perplex will consider.
12. When BUILD asks if you want to treat solution phases, say yes, and accept the default solution model file name.
13. There will be a whole bunch of "... solution will not be considered" lines, because many solution end-members are not present in the $H_2O-SiO_2-Al_2O_3-K_2O-MgO-FeO$ system.
14. When it asks you to select phases from the list, these are various solution models for different minerals. Many minerals have more than one possible model you could choose. For simplicity, we'll choose all the Holland & Powell models, plus hCrd for cordierite. Here is the list:

TiBio (HP)
Chl (HP)
Opx (HP)
Ctd (HP)
St (HP)
Gt (HP)
Sp (HP)
hCrd

15. Everything else should be as in tasks 1-3.

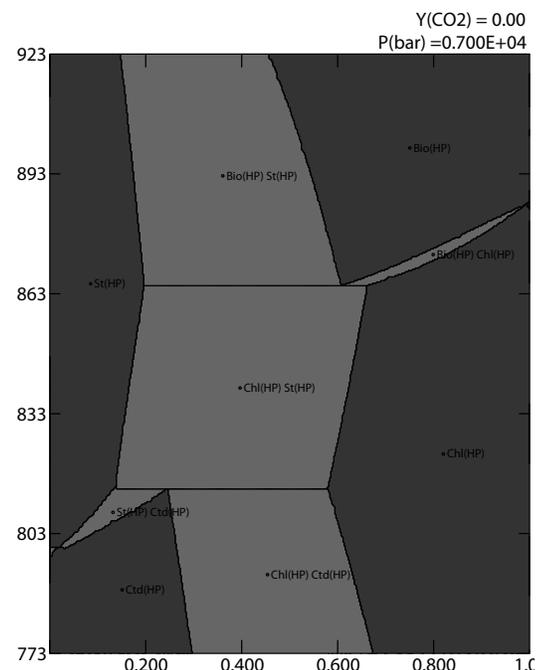
Results

Run VERTEX. It will take a while to run. Instead of a handful of phases whose free energies must be calculated, there are now thousands, because each solution phase is divided into a bunch of pseudocompounds. In addition, gridded minimization takes longer, but results in nice, smooth curves

Because the run used gridded minimization, we must plot the results with PSSECT instead of PSVDRAW. The plot should look like the figure at right.

Examine the print file. Most of it is made up of a list of the pseudocompounds and their MgO compositions (in mole fraction MgO), but near the end of the file, you will find a list like this:

Phases on saturation and buffering surfaces:



| | | | | | | |
|-------|------|------|------|-------|-------|-----|
| q | trd | crst | coe | stv | qL | qGL |
| q8L | and | ky | sill | tpz | prl | kao |
| cor | dsp | silL | coGL | sil8L | mu | mic |
| san | kals | lc | kspL | kal3o | kalo2 | k2o |
| kalGL | kcym | | | | | |

Question III-1: What do these phases have in common, and why are they listed here?

Question III-2: What do the colors in the diagram correspond to?

To help answer the next question(s) you might want to figure out exactly what is stable at a given T-X(Mg) condition. For this, you can use WERAMI. You should choose to compute properties at specified conditions, option 1.

Question III-3: What changes in a rock as it moves (conceptually) across the Chl + St field from left to right? (don't say X_{Mg}) From top to bottom? (don't say T)

Question III-4: How do the changes across a curved, steep boundary compare to changes across a horizontal field boundary? In other words, what do these lines signify?

Question III-5: Write the full balanced reaction across the lower horizontal boundary (at about 814K), including the phases you are projecting from. You can assume that the projected phases are quartz, kyanite, and muscovite, and you can express a change in the composition of a phase as two separate phases, a reactant composition and a product composition (like "Grt1" and "Grt2"). You will need to use WERAMI or MEEMUM for this, to get the assemblage just below and just above the reaction.

Task 6 - Making an AFM diagram

Now that we have some exposure to solid solutions, we'll try something a little more ambitious: the AFM diagram projected from muscovite. The reason this is challenging is that Perplex cannot truly plot components below the FeO-MgO join, so we have to "trick" it by changing the system components from FeO and MgO to $Fe_{0.75}Al_{-0.25}$ and $Mg_{0.75}Al_{-0.25}$. This will allow biotite to plot inside the new, larger triangle.

Building the run file

1. Choose a different name than last time, perhaps "task6"
2. This time, we'll say yes to transform the components. We need to transform three components. The first is K_2O , which we'll replace with $0.5K_2O + 1.5Al_2O_3$. This is the formula for muscovite (after projecting from water and quartz). This will be one of our components. This step is just the regular projection from muscovite. Here is the interaction:

The current data base components are:

```
NA2O  MGO  AL2O3  SI02  K2O  CAO  TIO2  MNO  FEO  NIO  ZRO2  CL2
O2    H2O  CO2
```

Transform them (Y/N)?

Y

Enter new component name, < 6 characters, left justified:

KprMs (this can be whatever you want other than a regular oxide name)

Enter old component to be replaced with KprMs:

K2O

Enter other components (< 14) in K 1 per line, <cr> to finish:

projection phases outside the diagram). Clean up the overlapping text to make a nice-looking plot, such as you might see in a textbook. Use regular mineral and end-member names or obvious abbreviations. This should be separate from the unimproved set of 6 plots.

Question III-6: Describe qualitatively the changes occurring from 773 K through 833 K. If you wanted to get more specific knowledge of these changes, how would you use Perplex to figure those out?

Question III-7: Identify two discontinuous reactions that must occur somewhere between 833 and 853 K.

Question III-8: Give the exact predicted composition (as proportions of end-members) of all minerals stable in this system at 5 kbar, 813 K, and $X(\text{CO}_2)=0$ in a rock whose bulk composition plots in the large low-Al, Fe-rich 3-phase triangle. You will have to look in the `task6_pseudocompound_list.txt` file for compositions, and you might need to put the file in an editor to read the labels which probably overlap each other. In addition, you will need the composition of the end-members listed in the pseudocompound glossary – you must use the compositions listed in `hp02ver.dat`, not those you find anywhere else (including textbooks).

Turn in your three plots (task 5, task 6, and the prettified version of the 560°C task 6 AFM plot) along with the answers to questions III-1 through III-8.

Perplex Tutorial IV: Pseudosections

You will recall that a pseudosection is a diagram showing the position of the various reactions in (generally) P–T space, customized for a particular bulk composition. These are very useful for a kind of rough thermobarometry. Note that there is an exhaustive tutorial on pseudosections on the Perplex website: http://www.perplex.ethz.ch/perplex_pseudosection.html

Task 7 - Mineral stability calculation for a pelite.

Here we will calculate the expected mineral stability for a simplified pelite. At right are bulk compositional data. These do not sum to 100%; the remainder is presumably H₂O and CO₂.

A full-blown pseudosection can take a long time (hours to days) to calculate. We'll make a problem file in build that we can use for making a pseudosection, but we'll start by calculating the stable phases at a particular P&T, somewhat like we did in task 1. We will assume that quartz is present, along with a water-rich (but impure) fluid.

| Oxide | Abundance (wt. %) |
|--------------------------------|-------------------|
| SiO ₂ | 56.36 |
| Al ₂ O ₃ | 14.454 |
| CaO | 4.0094 |
| FeO | 9.7741 |
| MgO | 4.4269 |
| MnO | 3.8721 |
| K ₂ O | 3.2427 |

Building the run file

1. Choose a different name than last time, perhaps "task7"
2. This time, perform the calculations with a saturated H₂O-CO₂ fluid phase, with the composition X(CO₂)=0.05, so list both H₂O and CO₂ as saturated phase components.
3. Assume that quartz, is present throughout, and thus requires saturated SiO₂.
4. The thermodynamic components should be all the non-SiO₂ oxides in the above table.
5. Choose gridded minimization.
6. Set the x-axis to be temperature from 450-700 °C, and the y-axis to be pressure from 5.0-7.5 kbar, and X(CO₂)=0.05 (so nearly pure water).
7. Do constrain the saturated components (SiO₂).
8. Agree to specify by weight (you can also specify by moles), and enter the amounts listed in the table for the various components.
9. Use these solution models:
 - TiBio (HP)
 - Chl (HP)
 - Opx (HP)
 - Cpx (HP)
 - Ctd (HP)
 - St (HP)
 - Gt (HP)
 - Sp (HP)
 - hCrd
 - feldspar
 - Pheng (HP)
 - M (HP)
10. Everything else should be as in tasks 1-3.

Results

Run MEEMUM. You do not want to interactively enter bulk compositions. You should perform the calculation at 700 °C, 7.0 kbar, and $X_{\text{CO}_2}=0.05$.

Question IV–1. What precise phases are stable for this bulk composition at these conditions? Give their compositions (as chemical formulae) and volumetric abundances, normalized to 100%.

Task 8 - P-T Pseudosection

Well, now you've got some idea of what to expect for this rock at some particular set of conditions (perhaps peak-T conditions for the area), but what about its history? That's where the pseudosection comes in handy. Let's say you were interested in finding out at what temperature garnet began to grow in this rock, and how much grew over time, or perhaps the order of mineral formation. Perhaps you are interested in how things might have been different if the fluid composition changed. All these questions can be answered with pseudosections.

Building the run file

1. Don't run build, because the build file is the same as in task 7. Just duplicate the task folder as task 8, change the name of the build file to "task8.dat", and edit its contents to change the names to reflect task 8 instead of 7.

Results

Run VERTEX. It should take a 3–30 minutes to run, depending on the speed of your computer. Run PSSECT to see the plot.

Annotate the pseudosection (using Illustrator or Inkscape) to show the line that separates garnet-bearing rocks from non-garnet-bearing rocks. (Note that some of the tiny regions are artifacts of the coarse resolution of the calculations and the line should just run through the middle of these tiny regions.)

PSSECT has great features that allow us to see very clearly where the fields are that contain a particular assemblage. Suppose we have a rock with the assemblage Grt+Bt+Chl+Qtz+Fsp, along with other phases we haven't yet identified; let's see how PSSECT can help us. First make a duplicate of the postscript file that you just made, and name the duplicate something like "task8plotA.ps". (We do this because otherwise PSSECT will overwrite your file with a new one of the same name.) Now run PSSECT again, and when it asks you if you want to modify the default plot, say yes:

```
Modify the default plot (y/n)?
```

```
y
```

```
Modify drafting options (y/n)?
```

```
answer yes to modify:
- x-y plotting limits
- axes numbering
```

```
n
```

```
Restrict phase fields by phase identities (y/n)?
```

```
answer yes to:
- show fields that contain a specific assemblage
- show fields that do not contain specified phases
```

- show fields that contain any of a set of specified phases

y

WARNING: You can not specify saturated phases or phases determined by component saturation constraints in these restrictions.

Show only with assemblage (y/n)?

y

Enter the name of a phase present in the fields
(left justified, <cr> to finish):

Gt (HP)

Enter the name of a phase present in the fields
(left justified, <cr> to finish):

TiBio (HP)

Enter the name of a phase present in the fields
(left justified, <cr> to finish):

Chl (HP)

Enter the name of a phase present in the fields
(left justified, <cr> to finish):

feldspar

Enter the name of a phase present in the fields
(left justified, <cr> to finish):

Show only without phases (y/n)?

n

Show only with phases (y/n)?

n

There are 6 fields for: Chl(HP) Pheng(HP) feldspar Gt(HP) TiBio(HP) zo q
60336 fields have the assemblage: Gt(HP) TiBio(HP) Chl(HP) feldspar

Examine the new plot.

Question IV-3. What additional mineralogical information would you need from the rock to determine in which of the fields it falls (presuming you know it falls in this region of P-T-X(CO₂) parameter space)?

Question IV-4. Why didn't we specify quartz to pssect as one of the minerals? How did it still find quartz (see "q" in the last lines of its output)?

You can also calculate how much garnet has formed at any given condition, by making a property grid with WERAMI and then plotting it with PSTABLE. Make another copy of the postscript file to preserve it (task8plotb.ps), and run WERAMI:

Enter the project name (the name assigned in BUILD) [default = my_project]:

task8

Reading computational options from: perplex_option.dat

Writing computational option summary to file: not requested

[Shows options settings. The only important one to note is the proportions setting, which dictates whether the proportions of phases are based upon mass, volume, or moles:]

Perple_X computational option settings for WERAMI:

| Keyword: | Value: | Permitted values [default]: |
|----------|--------|-----------------------------|
|----------|--------|-----------------------------|

Input/Output options:

| | | |
|----------------|-----|-----------------|
| spreadsheet | T | [F] T |
| logarithmic_p | F | [F] T |
| bad_number | NaN | [0.0] |
| composition | mol | wt [mol] |
| proportions | vol | wt [vol] mol |
| interpolation | on | off [on] |
| melt_is_fluid | F | [F] T |
| seismic_output | som | none [some] all |

Information file output options:

| | | |
|-------------------|---|-----------------------------------|
| option_list_files | F | [F] T; echo computational options |
|-------------------|---|-----------------------------------|

Thermodynamic options:

| | | |
|--------------------|---|-------|
| approx_alpha | T | [T] F |
| Anderson-Gruneisen | F | [T] F |

Seismic velocity options:

| | | |
|-----------------------|-----|-------------------------------------|
| bounds | VRH | HS [VRH] |
| vrh/hs_weighting | 0.5 | 0->1 [0.5] |
| explicit_bulk_modulus | T | [F] T |
| poisson_ratio | on | off [on] all; Poisson ratio = 0.35 |

To change these options see: www.perplex.ethz.ch/perplex_options.html

Select operational mode:

- 1 - properties at specified conditions
- 2 - properties on a 2d grid
- 3 - properties along a 1d path
- 4 - as in 3, but input from file
- 0 - EXIT

2

Select a property [enter 0 to finish]:

- 1 - Specific Enthalpy (J/m3)
- 2 - Density (kg/m3)
- 3 - Specific heat capacity (J/K/m3)
- 4 - Expansivity (1/K, for volume)
- 5 - Compressibility (1/bar, for volume)
- 6 - Composition (Mol or Wt%) of the system
- 7 - Mode (Vol, Mol, or Wt proportion) of a phase
- 8 - Composition (Mol or Wt%) of a solution phase
- 9 - Grueneisen thermal ratio
- 10 - Adiabatic bulk modulus (bar)
- 11 - Adiabatic shear modulus (bar)
- 12 - Sound velocity (km/s)
- 13 - P-wave velocity (Vp, km/s)

- 14 - S-wave velocity (V_s , km/s)
- 15 - V_p/V_s
- 16 - Specific entropy (J/K/m³)
- 17 - Entropy (J/K/kg)
- 18 - Enthalpy (J/kg)
- 19 - Heat Capacity (J/K/kg)
- 20 - Specific mass of a phase (kg/m³-system)
- 21 - Poisson ratio
- 22 - Molar Volume (J/bar)
- 23 - Dependent potentials (J/mol, bar, K)
- 24 - Assemblage Index
- 25 - Modes of all phases
- 26 - Sound velocity T derivative (km/s/K)
- 27 - P-wave velocity T derivative (km/s/K)
- 28 - S-wave velocity T derivative (km/s/K)
- 29 - Adiabatic bulk modulus T derivative (bar/K)
- 30 - Shear modulus T derivative (bar/K)
- 31 - Sound velocity P derivative (km/s/bar)
- 32 - P-wave velocity P derivative (km/s/bar)
- 33 - S-wave velocity P derivative (km/s/bar)
- 34 - Adiabatic bulk modulus P derivative (unitless)
- 35 - Shear modulus P derivative (unitless)
- 36 - All phase &/or system properties
- 37 - Absolute amount (Vol, Mol, or Wt) of a phase
- 38 - Multiple property output
- 39 - Heat capacity ratio (C_p/C_v)

7

Enter solution or compound name (left justified):

Gt (HP)

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select a property [enter 0 to finish]:

0

Change default variable range (y/n)?

n

Enter number of nodes in the x and y directions:

200 200

****warning ver637**** Immiscibility occurs in one or more phases
interpolation will be turned off at all affected nodes.
To override this feature at the risk of computing inconsistent properties
set solvus_tolerance = 1 and rerun VERTEX

Data ranges excluding values equal to bad_number (NaN) specified in perplex_option.dat:

```

      Gt (HP), vo%
min    0.2614957
max    30.42436

```

Output has been written to the 2d tab format file: task8_1.tab

(Note here that WERAMI is smart enough to not overwrite existing files, and instead appends a number to the end.)

2d tab format files can be processed with:

```
PSTABLE - a Perple_X plotting program
PERPLE_X_PLOT - a MATLAB plotting script
PYWERAMI - petrol.natur.cuni.cz/~ondro/pywerami:home
spread-sheet programs, e.g., EXCEL
```

for details on tab format refer to:

```
perplex.ethz.ch/faq/perple_x_tab_file_format.txt
```

Select operational mode:

```
1 - properties at specified conditions
2 - properties on a 2d grid
3 - properties along a 1d path
4 - as in 3, but input from file
0 - EXIT
```

0

Now run PSTABLE to make the actual plot:

Enter the tab file name [without the .tab suffix]:

task8_1

Plot the ratio of two dependent variables (Y/N)?

N

Select the dependent variable to be contoured:

```
1 - T(K)
2 - P(bar)
3 - Gt(HP),vo%
```

3

****warning ver004**** the data includes NaN values, probably because bad_number in perplex_option.dat = NaN, these values will be replaced by zeros. To avoid this behavior set bad_number to a numeric value or use a plotting program capable of handling NaNs, e.g., MatLab or PYWERAMI

Contour the ratio of values in separate tab files (y/n)?

If you answer yes the data from the file just read will define the numerator of the ratio and you will be prompted next for a file containing the data for the denominator.

N

PostScript will be written to file: task8_1.ps

Modify the default plot (y/n)?

N

```
Contoured variable range:    0.00000    ->    30.4244
Range excluding zero values:  0.261496    ->    30.4244
```

Modify default contour interval (y/n)?

Y

Enter min, max and interval for contours:

3 33 3

Echo contour data to file contor.dat (Y/N)?

N

Examine the new plot (task8_1.ps). Note that it's pretty tough to figure out what numerical value each contour represents. Consider how you could figure it out easily with the tools you've learned so far.

Question IV-5. Describe what would happen to garnet if the rock were to be isobarically heated at 7 kbar over this temperature range?

Finally, you can determine the composition of the garnet being produced. Redo WERAMI and PSTABLE as above, but this time choose property 8 - the composition of a solution. Here we'll plot the MnO content of the garnet.

1. Choose property 8, and enter the garnet solution model.
2. We'll plot MnO. Select one component in the numerator, MNO (with a weighting value of 1), and give 0 for the denominator (nothing in the denominator):

Compositions are defined as a ratio of the form:

$$\frac{\text{Sum } \{w(i)*n(i), i = 1, c1\}}{\text{Sum } \{w(i)*n(i), i = c2, c3\}}$$

n(j) = mole proportion of component j
w(j) = weighting factor of component j (usually 1)

How many components in the numerator of the composition (<13)?

1

Enter component indices and weighting factors for the numerator:

- 1 - AL2O3
- 2 - CAO
- 3 - FEO
- 4 - MGO
- 5 - MNO
- 6 - K2O
- 7 - SIO2
- 8 - H2O
- 9 - CO2

5 1

How many components in the denominator of the composition (<15)?

Enter zero to use the numerator as a composition.

0

The compositional variable is: 1.0 MNO

Change it (y/n)?

N

This composition will be designated: C1Gt(HP)

3. Contour the whole range.

Plot the results with PSTABLE, using a contour interval of 0.1 with a range from 0.1-1.3. Examine the new plot.

Annotate this plot (task8_2.ps) to label the contours.

Question IV-6. Describe the MnO of the garnet during isobaric heating at 7 kbar. We know that garnet often has high Mn values in its core and smoothly decreasing Mn content toward the rim. Does that match with what the you would predict from this pseudosection? If not, how can you reconcile the two?

- Turn in four plots (task 8 full pseudosection with Grt annotation, pseudosection showing Grt+Bt+Chl+Qtz+Fsp regions, garnet mode plot, annotated garnet MnO plot), each with an informative title, along with the answers to questions IV-1 through IV-6.**

Advanced Perplex Assignment

Now that you have learned how to use Perplex, here is your main assignment: You will calculate one or more diagrams to illustrate some aspect of metamorphic petrology. Here are some ideas:

- You might take a rock you have already analyzed with petrography, EPMA or quantitative SEM-EDS, and XRF, and make a pseudosection of it, then try to figure out where on the pseudosection your rock falls, based on assemblage, mineral modes, and mineral chemistry. Also try to see if your textures make sense with the pseudosection. (For Dave's class, this will be PR3 in the term project; don't do a separate advanced assignment).
- You might take a bulk composition and a metamorphic field gradient, and calculate the evolution of mineral assemblage and composition along the field gradient. Creating a set of appropriate ternary diagrams for points along the path would be a useful addition.
- You might take a bulk composition and a P-T path and calculate the evolution of mineral assemblage and composition along the path. Creating a set of appropriate ternary diagrams for points along the path would be a useful addition.
- You might calculate parallel pseudosections for a set of different rock compositions to document the relation between reactions found in each one at some reasonable condition. You should select a set of compositions that might plausibly be found together in a protolith package (e.g., ultramafic and laterite would not typically be found together).

Model bulk compositions for pelites can be found here: Shaw, D. M. (1956) Major elements and general geochemistry, Part 3 of Geochemistry of pelitic rocks, *Geological Society of America Bulletin*, vol.67, no.7, pp.919-934. Other sedimentary and igneous bulk chemical analyses can be found on the web or in journal articles, but here are two easy sources:

- http://minerals.cr.usgs.gov/geo_chem_stand/
- <http://www.aist.go.jp/RIODB/geostand/>

You will give a brief presentation on your results in class.