

## introduction to drawpd (for dr118, Feb 2020)

**Drawpd** is software that takes manually-assembled mode-1 THERMOCALC output and produces an encapsulated postscript (eps) rendering of the resulting phase diagram. You need an appropriate THERMOCALC axfile and scriptfile to run THERMOCALC to get the necessary output. The THERMOCALC scriptfile needs to include the script (keyword), **drawpd**, on its own line. When a calculation is done that contributes to the pseudosection—for example a `mode=0` line, bounding a field in the pseudosection—THERMOCALC writes the output in **drawpd** form in `tc-x-dr.txt`, where `x` is the part of the THERMOCALC scriptfile name, `tc-x.txt`. In `tc-x-dr.txt` is the information to be copied into the **drawpd** datafile. The name of the **drawpd** datafile can be anything of the form, `dr-blah.txt`, but conventionally it is `dr-x.txt`, matching the corresponding THERMOCALC filenames. When **drawpd** is run with `dr-x.txt`, the encapsulated postscript output file produced will then be called `dr-x.eps`, with the **drawpd** log file called `dr-log.txt`, summarising the work that **drawpd** has done (helping for example with debugging datafiles).

In the THERMOCALC scriptfile, the script, **drawpd**, may be followed by an optional code, currently 0 or 1 (0 is the default). **Drawpd** 0 results in lines and points just involving  $P$  and  $T$  information in the `tc-x-dr.txt`. **Drawpd** 1 results in lines and points involving  $P$  and  $T$ , and as well  $G$ ,  $H$ ,  $S$ ,  $V$  and  $\rho$  information ( $G$  is Gibbs energy, etc, and  $\rho$  is density). This allows contouring for these properties (currently by Mathematica code, but, in the future, in **drawpd** itself). Additional codes will be implemented in future, for example, allowing inclusion of modes and site fractions in the output for **drawpd**. The output in **drawpd** form in `tc-x-dr.txt` is also given in comma-separated form (csv) in `tc-x.csv` for those wishing to plot diagrams their own way.

Building up a pseudosection line-by-line, you need to copy the relevant parts of the `tc-x-dr.txt` file into the `dr-x.txt` file each time you exit THERMOCALC. When THERMOCALC is started again the contents of the `tc-x-dr.txt` file is overwritten. If you are new to calculating pseudosections, or if the pseudosection is unknown or at all tricky, it is worthwhile running THERMOCALC and sketching (on paper) the phase relations for each part of the diagram, before then rerunning the calculations to collect the **drawpd** information. It is what I usually do.

The information copied into the `dr-x.txt` file requires a small amount of editing before **drawpd** is run, as outlined below. Also, in addition to the blocks of information for each equilibrium, instructions that control the behaviour of **drawpd** are included in the **drawpd** datafile.

You should learn a lot by correlating what is in the  $PT$  pseudosection in Fig. 1 with the information in the datafile used by `drawpd` to draw it, in `dr-fig4.txt`. Some key parts of the datafile are copied below. The datafile is provided with this pdf as a textfile so you can run it in `drawpd` yourself, playing with the scripts to see the effect they have on the diagram produced. The information in the datafile is sufficient to draw the diagram for a much larger range of  $PT$  (0.5 to 12 kbar, and 630° to 1000°C)

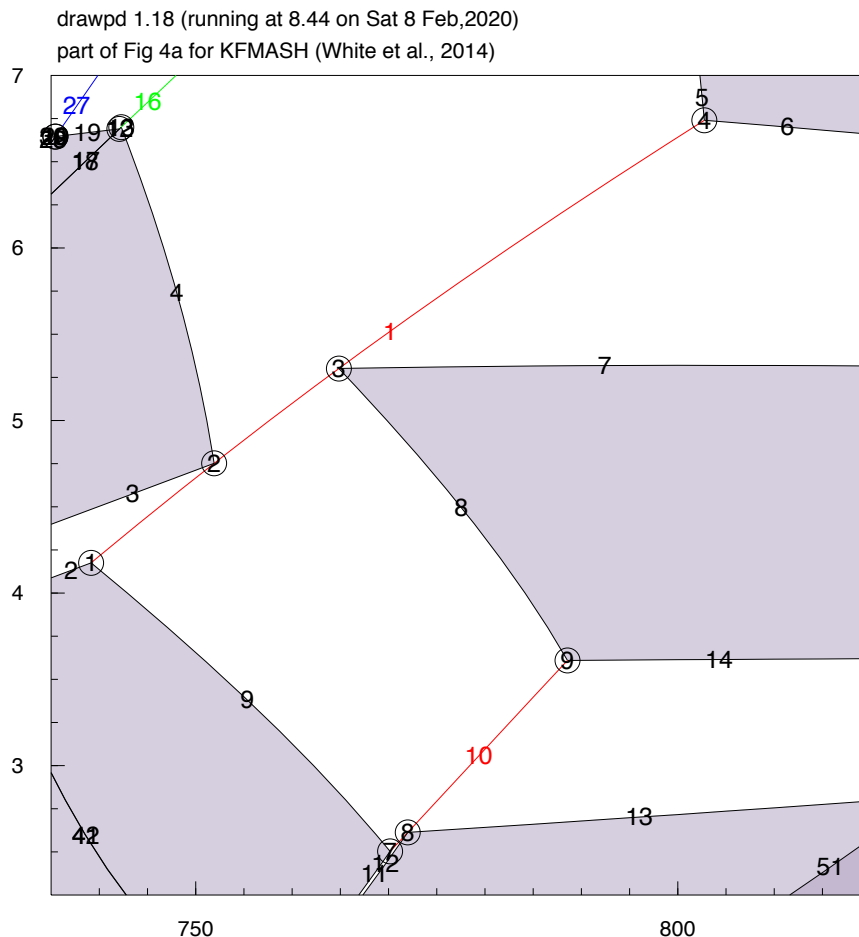


Figure 1: A blowup of a  $PT$  range of the pseudosection in Fig. 2, as calculated and drawn by `drawpd` using the datafile, `dr-fig4a.txt`, generated by Richard White. The numbers on the lines correspond to the `u` info in the datafile, e.g. line 8 is `u8` in the datafile. The numbers in the circles correspond to the `i` info in the datafile, e.g. point 3 is `i3` in the datafile. Line 1 is the AFM univariant,  $bi + sill = g + cd$ , and line 10, the univariant,  $bi + g = opx + cd$ , both with  $+q+ksp+liq$ . See Fig.2, below, for the labelling of the fields. This is the diagram as produced by `drawpd` from `dr-fig4a.txt`; it is not cleaned up in any way.

In looking at the contents of `dr-fig4.txt`, the first thing to note is that anything after a “`%`” is a comment (as in THERMOCALC datafiles). Comments annotate what is in the datafile, with some created by THERMOCALC, some added for this documentation, but you may add

your own comments as appropriate.

The overall **drawpd** datafile structure involves four sections which **drawpd** uses:

1. initial setup (e.g which columns of the data are  $x$  and  $y$  on the requested diagram)
2. the description of the points/lines (THERMOCALC output), terminated by a “\*”
3. definition of areas to be shaded/coloured, terminated by a “\*”
4. scripts controlling a phase diagram’s “window” etc, terminated by a “\*”
5. storage area (not read by **drawpd**)

More information on each of these sections follows now.

**1. initial setup** in `dr-fig4a.txt`, it is self-explanatory with the annotation:

```
2      % no of numbers in each line of data, in this case 2, P and T
6      % system size - in this case KFMASH with 6 components
2 1    % which columns to be x,y in phase diagram: so x = T, y = P in this case
```

The number of numbers in each line of data is controlled by the scriptfile when THERMOCALC is run. The script, **drawpd**, has an optional code controlling what information is output for calculated equilibrium (see above).

For some diagrams, e.g.  $T$ - $x$  ones, THERMOCALC cannot (currently) calculate points directly. In this case there is a **drawpd** script, **x**, that allows interpolation to find such points. If, for example, there are 3 numbers per line,  $\{x, P, T\}$ , and a  $T$ - $x$  diagram at  $P = 5$  kbar is being drawn, then calculation in THERMOCALC of the point-defining equilibrium at a series of pressures through 5 kbar—defining a  $x$ - $P$ - $T$  locus of the equilibrium—is used by **drawpd** to get the coordinates of the point at 5 kbar. The script for this example is

```
x 2 5 % interpolation, in this case for the 2nd variable (P) at 5 kbar
```

**2. points and lines** This section just contains information copied out of the `tc-x-dr.txt` file into the `dr-x.txt` file, with a few edits. For points, the THERMOCALC output, for example for the point on the `bi+sill=g+cd` univariant where the modes of `bi` and `sill` are zero, looks like

```
i<k>    g cd liq ksp q  - bi sill
5.301 764.85 % bi = 0, sill = 0
```

The one edit required for point information is that <k> must be replaced by a number (or any characters) of your choice (no spaces). This is then used for labelling. So, after editing, this became, as in the file<sup>1</sup>, including added annotations

```
i3  g cd liq ksp q  - bi sill      % ie calc with g cd liq ksp bi sill, with
                                     % the modes of bi & sill set to zero
5.301 764.85  % bi = 0, sill = 0
```

For lines, there are several edits necessary and/or optional. The first corresponds to that for points, replacing <k>, as done here

```
u8  g cd liq ksp q  - bi
```

```
begin end
```

```
3.400 790.60  % bi = 0
3.600 788.66  % bi = 0
3.800 786.51  % bi = 0
...
```

As the phase diagram is built up (usually sketched on paper), it is seen that u8 runs from i9 to i3, to give what is in the **drawpd** datafile:

```
u8  g cd liq ksp q  - bi
```

```
i9  i3                                     % plot line between i9 and i3
```

```
3.400 790.60  % bi = 0
3.600 788.66  % bi = 0
3.800 786.51  % bi = 0
...
```

Plotting with respect to the bounds of the diagram are handled automatically via the **window** specification in section 4, described below.

After the line-limit specification, certain keywords may appear, controlling how the line is plotted. These include **red** (as for univariant u1 in the datafile), **blue**, **green**, **magenta**, **thick** and **dashed**.

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<sup>1</sup>The results in **dr-fig4.txt** were calculated with **tc347**. The results with **tc350** and current files are slightly different, e.g. the coordinates of this point are {5.338, 765.66} with datafiles at (7-2-20).

Colour can also be specified using the keyword, **rgb**, followed by three integers representing r g and b (see the THERMOCALC script documentation for automatic colouring, for example making red all g-out lines in a pseudosection).

For short lines between points on a pseudosection, there is a keyword, **connect**, that can be used to draw such lines. For example in the datafile, look for **u70**<sup>2</sup>. Another keyword, **crossover**, can be used to define a point in terms of crossing lines. For example in the datafile, look for **i9**.

3. **areas** This section of the datafile concerns colouring of areas (fields) in pseudosections. This is done by specifying the boundary lines of each field, in order, as can be seen in **dr-fig4.txt**. An example is

```
0.8 u7 u8 u14 u58
```

The first number relates to the colour to use for the field. For white, this is 1. For a number less than 1, this is a factor giving a colour between white and a “dark colour” as specified in the **darkcolour** specification in section 4, described below. Using 0, means that the dark colour itself is used for the field. Then the boundary lines are listed

4. **scripts** The mandatory scripts in this section concern the “window” of the phase diagram, and the *x* and *y* values associated with the number labelling of the axes.

```
window  735 820 2.25 7    % plot window, in this case Tlow, Thigh, Plow, Phigh

bigticks  50 750 1 3      % main ticks and labelling, in this case
                        %      every 50 starting at 750C, and
                        %      every 1 kbar starting at 3 kbar
```

With the annotation, the meaning of these is self-explanatory. A way to think about the window is that there is a (much) bigger phase diagram that has been calculated, but that via the **window** keyword, a part of that bigger diagram can be looked at. Looking at such different parts of the diagram just involves changing the 4 numbers following the **window** keyword.

The keyword, **bigticks**, controls where the number labels appear on the axes of the phase diagram, and where the big ticks are on those axes. You need to adjust these as you adjust the window.

Optional scripts include **smallticks** (small ticks between the big ticks), **info** (line or lines with text that is printed above the diagram), **darkcolour** (with three numbers for

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<sup>2</sup>in this case the assemblage involved is not given, nor the mode=0 phase. In the future this information may be required, rather than being effectively optional, as implied here

r g and b, giving the colour scheme of the diagram), **numbering** (the u numbers from the datafile are printed on the lines in the diagram, with a font size given by the number following the script), and **circles** (the i numbers from the datafile are printed on the points in the diagram, within circles, of radius specified). An example of the use of these scripts, taken from the datafile, dr-fig4.txt, is

info part of Fig 4a for KFMASH (White et al., 2014)

```
smallticks 5 0.25      % minor ticks, in this case T,P, starting at Tlow and Plow
darkcolour 56 16 101   % red green blue in 0<->255, as in Illustrator RGB
numbering 14            % numbering the lines on the diagram
docircles 7            % add numbers and circles for points on the diagram
```

The best way to investigate what drawpd can do is to change the scripts in the example datafile and rerun drawpd. In the storage area of the datafile are some possibilities.

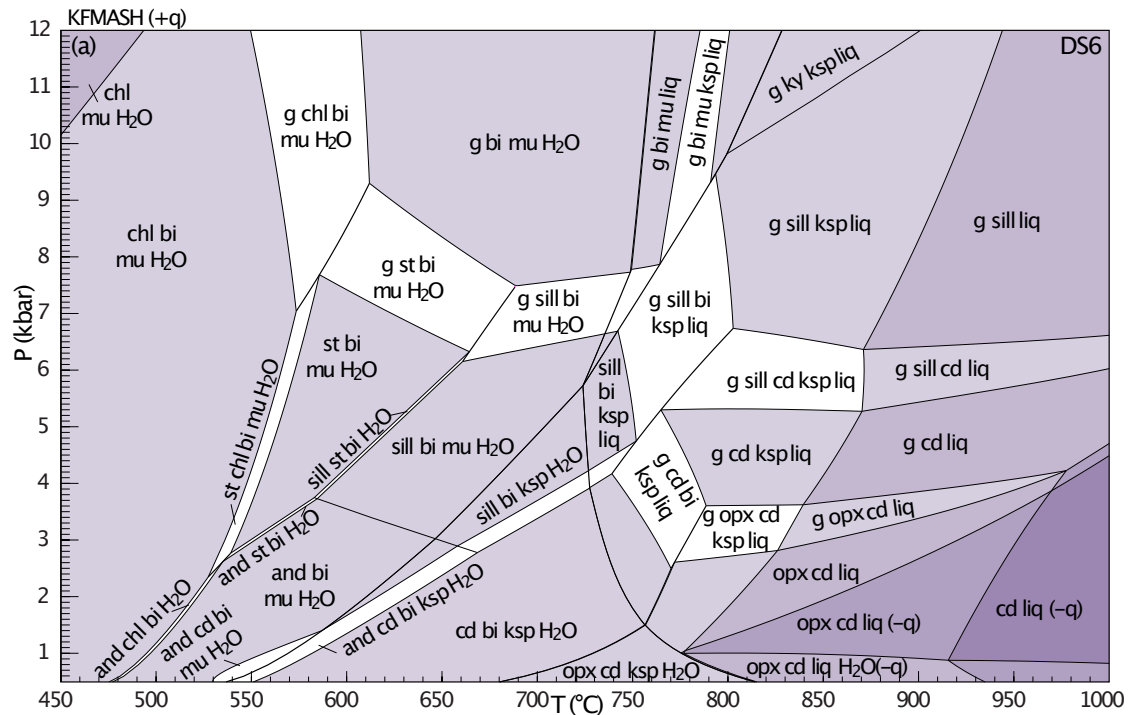


Figure 2: A labelled version of the  $PT$  pseudosection of which Fig. 1 is a blowup. It is Fig. 4a in White *et al.* (2014, *JMG*, **32**, p.269), in KFMASH for a bulk composition given there.