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PP: A Graphics Post-Processor for the EQ6 Reaction Path Code

H. W. Stockman

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PP: A GRAPHICS POST-PROCESSOR FOR THE EQ6 REACTION PATH CODE

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Abstract

The PP code is a graphics post-processor and plotting program for EQ6, a popular reaction-path code. PP runs on personal computers, allocates memory dynamically, and can handle very large reaction path runs. Plots of simple variable groups, such as fluid and solid phase composition, can be obtained with as few as two keystrokes. Navigation through the list of reaction path variables is simple and efficient. Graphics files can be exported for inclusion in word processing documents and spreadsheets, and experimental data may be imported and superposed on the reaction path runs. The EQ6 thermodynamic database can be searched from within PP, to simplify interpretation of complex plots.

Acknowledgments

The author thanks Jim Garner and Christine Stockman of Sandia Dept. 6342 for testing the many versions of PP, and Thomas J. Wolery of Lawrence Livermore National Laboratory for helpful advice and the chance to use EQ6.

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1. Introduction

The EQ6 reaction path code (Wolery, 1992) uses thermodynamic and kinetic data to predict the chemical evolution of systems containing water, rocks and soils, and man-made materials (Bruton and Shaw, 1988; Gardiner *et al.*, 1989; Criscenti and Arthur, 1991). EQ6 is a powerful and flexible tool, but like any reaction path code, it tends to overwhelm the user with information. A single reaction path run may generate concentration and saturation state data for hundreds of aqueous species and mineral phases, sampled over several hundred steps. The ASCII tables produced by EQ6 are well-organized, and generally sample only the most significant portions of the reaction path (typically fewer than 20% of the calculated steps); nonetheless, these tables can be several megabytes in size, and analysis of the results can be an intimidating prospect for all but the very experienced user. Increasingly, EQ6 is applied to problems of waste disposal and environmental modeling, and the calculations must be performed by users with little experience in reaction path modeling or computational chemistry.

The program PP is a simple but flexible graphics post-processor for EQ6. PP provides a "point and click" environment for plotting the results of reaction path runs, for exporting the results to spreadsheet files, CAD and word processing programs, and for exploring the EQ6 thermodynamic databases. PP was written to make EQ6 accessible to a wider range of investigators, particularly "occasional" users with some understanding of aqueous chemistry, but modest knowledge of the computing environment. By using a compact binary input file, PP can preserve data from all steps calculated by EQ6. This report provides instructions for installing PP on a personal computer, a tutorial, and documentation of more advanced capabilities.

1.1 Availability

The binaries for PP are available from the author (e-mail hwstock@sandia.gov), subject to the constraints indicated in the closing banner of the program, viz:

```
PP version 1.00  HW Stockman  08-07-94
```

```
=====
This program was prepared by Sandia National Laboratories (Contractor)
under contract No. DE-AC04-94AL85000 with the U.S. Department of Energy
(DOE). All rights are reserved by DOE on behalf of the Government and
the Contractor pursuant to the contract. You are authorized to use
this program for Government purposes but it is not to be released or
distributed to the public. Neither the Government nor the contractor
makes any warranty, express or implicit, or assumes any liability or
responsibility for the use of this software. Any copies made should
carry this notice.
```

The EQ3/6 code suite is copyrighted by the University of California, and is independent of PP. Instructions for obtaining EQ3/6 can be found in the EQ3/6 manuals (Wolery, 1992). Currently, the Energy Science and Technology Software Center in Oak Ridge, TN (615-576-2606) handles distribution of EQ3/6. The appendix of this report describes the function that must be added to EQ6 to produce the binary plot files read by PP.

1.2 Installing PP on a Personal Computer

PP runs under DOS on "IBM-compatible" computers based on Intel 486DX, 486SL or Pentium, and compatible processors. The computer should have at least 4 MB of free hard disk space and 2 MB of RAM, and a video adapter (graphics card) capable of supporting at least 16 colors at a resolution 640x480 pixels. The program will run on 386-based computers with an 80x87-compatible math coprocessor, but performance may be unacceptable. If PP is used to search the EQ6 databases, the computer should have at least 4 MB, and preferably 8 MB RAM. PP contains its own DOS-extender, runs in 386 protected mode, and allocates memory dynamically as needed. PP can also run full-screen under Microsoft Windows 3.1, and several copies of the program can be active at once, operating on different data sets.

To install PP, first create a directory called `\pp` on the hard drive by typing the following sequence of commands at the DOS prompt:

```
c: ↵  
cd \ ↵  
md pp ↵
```

where the "↵" represents the "Enter" key. Then enter the directory by typing:

```
cd pp ↵
```

Now copy the distribution file onto the hard disk:

```
copy a:pp4eq6.exe c:\pp ↵
```

If the floppy disk drive is called `b:`, substitute `b:` for `a:` above. Then type:

```
pp4eq6 ↵
```

which will extract the following files:

<code>pp.exe</code>	-- the main program;
<code>help_pp</code>	-- the on-line help file (section 3.3);
<code>external.fnt</code>	-- the "external" or triplex font file (section 5.10);
<code>ff.exe</code>	-- a simple font editor (section 5.10);
<code>hwsdata</code>	-- a sample data file, from the EQ6 <code>micro.6i</code> run;
<code>eq6_mods.for</code>	-- <code>eq6.for</code> modifications necessary to produce the <hwsdata> binary file (Appendix); and</hwsdata>
<code>t4a.6i, t4b.6i</code>	-- EQ6 input files for second part of tutorial.

To help PP find **help_pp** and the **external.fnt**, add the following line to the **autoexec.bat** file:

```
set PP=C:\pp
```

Note it is important to capitalize "PP=".

Like most reaction path codes, EQ6 uses mineral names to identify solid phases. Sometimes these names are quite peculiar (*e.g.*, mirabelite and haiweeite), and give no hint about the composition of the phase. PP has a facility to locate the composition, thermodynamic and reference data for these minerals, by searching the EQ3/6 database. To search the EQ3/6 database through PP, one should also set the **EQ36_DB** environment variable to point to the directory where the EQ3/6 **data0.*** files are stored. That is, a statement such as

```
set EQ36_DB=[drive]:\[path]
```

should be added to **autoexec.bat**. Typically the path will be **\eq3_6v7.2a\import** (see also Searching the EQ3/6 database, section 5.4).

Finally, add **\pp** to the path statement in **autoexec.bat**, so the computer will be able to find the executable files regardless of the working directory.

1.3 Starting the Program; Command-line Arguments

PP can be started ("invoked") by typing **pp** ← at the DOS prompt. However, PP can also be invoked with one or two optional command-line parameters:

pp [6|L|8|M] [filename] ←

The order of the two parameters is unimportant; that is, **[filename]** can appear first.

The **[6|L|8|M]** argument attempts to force a particular video mode. The "8" or "M" selection tries to force medium resolution, 800x600 pixel "superVGA" mode; *this is the preferred mode*, striking a balance between speed and resolution. The "6" or "L" selection tries to force low-resolution 640x480 pixel mode. If there is no **[6|L|8|M]** parameter, PP will attempt to pick the highest resolution supported by the computer's video hardware. Some LAP-TOP computers require the "6" switch; if PP is allowed to pick the "best" video mode, the screen may appear totally blank. If the computer has a VESA driver, it is often helpful to load this driver before running PP (consult the video card documentation for the name and location of the VESA driver; the name often contains the word "vesa"). Since graphics card technology is changing rapidly, it is safest to begin with the "**pp 6**" invocation. If PP comes up with an unreadable screen, press the Esc key, then the "Y" key to return to DOS.

The **[filename]** argument specifies an alternate name for the binary input file. The modified version of EQ6 (Appendix) produces a binary file named **hwsdata**, and by default PP looks for that file in the current directory. Each successive EQ6 run destroys the old **hwsdata** file. It may be desirable to save the results of previous runs by renaming the **hwsdata** files, or storing them in another location. The **[filename]** option makes it possible for PP to read these renamed files.

Here are some sample invocations and corresponding actions:

pp ←	PP reads hwsdata , starts at highest possible resolution;
pp 8 ←	PP reads hwsdata , starts at 800x600 pixel resolution;
pp 6 hwsdata.old ←	PP reads hwsdata.old , starts at 640x480 pixel resolution;
pp hwsdata.old L ←	Same as previous line (6=L, order unimportant).

PP has only two main screens: (1) the variables screen, entered first, which lists all the variables calculated by EQ6; and (2) the plot screen, which allows one to see, edit, and output x-y plots of elemental, mineral, fugacity and species concentration or saturation states. Both screens are mouse-aware, though one can perform nearly all actions with the keyboard by pressing the "hot keys" on the menu bars. Mouse-aware menu bars have a dark cyan (blue-green) background, with light cyan buttons (highlights). The hot keys are indicated by bright white letters on a dark red or green background. **NOTE** that one moves back and forth between the screens with the "PLOT" and "Varia" buttons. To exit the program, press the Esc key and then type 'Y'. The Esc key can also be used to "back out" from most of PP's menus and dialog boxes.

2. Tutorial

To begin the tutorial, switch to the directory that contains the **hwsdata** file and invoke PP by typing **pp 8** ← (preferred) or **pp 6** ← at the DOS prompt.

PP will come up in the **variables** screen. A small arrow (the **mouse cursor**) will move about the screen as the mouse is moved.

Figure 1. The variables screen.

Move the mouse cursor over the "minerals" icon and click the **left** mouse button. A lowercase 'y' will appear in the left-most column next to each mineral name, indicating that these variables have been selected for plotting on the left vertical axis (figure 1). If the right mouse button were clicked instead, uppercase 'Y's would appear, indicating the variables had been chosen to plot against the right vertical axis. If the computer lacks a mouse, press F4 to select all the minerals.

Now click on the **Plot** button, or press the 'P' on the keyboard. The plot screen appears, as shown in figure 2. Across the top of the screen is a row of light blue-green buttons with red and white highlights. Below the buttons are two reminders about mouse operations in the main plot screen: "left grabs label" and "right button=zoom". We will next use the left mouse button to move a label.

Note that the variables screen (figure 1) is divided into 7 vertical columns, labeled **yx1** to **C**. The entries in the right-most 5 columns affect the appearance of the plots, and can be altered by clicking the mouse button on each item, or by typing the highlighted letter on the keyboard. The variable to be altered is inside a purple bar cursor . Thus if we moved the bar cursor over the **Al++** row, and clicked repeatedly on the entry under the **L** column heading, the line type would toggle through , , and "none" choices. The same effect would be obtained by repeatedly typing 'L', the highlighted letter in "Line".

Figure 2. The plot screen.

The buttons that appear at the top of figure 3 can be used to alter the appearance of the labels and the associated curves. The first button on the left deletes the selected curve from the plot; the utility of this option is not obvious for so simple a plot, but it becomes important when one plots saturation states (Q/K) or species concentrations, where the plot may contain several hundred curves. The second changes the type of line used to connect the points on the curve; in figure 3, the current line type is "solid". The third button selects the symbol used to mark points on the curves, and the fourth selects the size of the text label; the fifth picks the curve color. The sixth button, labeled "What is this ???", searches the EQ3/6 database for information on the corresponding species or mineral, and displays the information; this button provides a scrollable window into the database (which may be several megabytes), with search capability.

Figure 3. Moving a curve label. Move the mouse cursor over the Muscovite label, and click once with the left mouse button. A dashed box will appear around the label, and a ghosted copy of the label is now attached to the mouse cursor. (Note that the curve associated with the label becomes highlighted in white; this highlight is quite helpful with complicated plots containing tens to hundreds of curves.) Move the mouse cursor down and left as shown in figure 3. Draw an arrow from the label to the nearest point on the curve by pressing 'A'. To erase the arrow, press 'E'. To fix the label in its new position, click the left mouse button again.

At this stage, one could continue to edit other curve and label characteristics, by clicking on other buttons (such as "Color") on the top menu bar. To return to the main plot screen, one could either (1) click a mouse button in the middle (gray) portion of the plot screen, or (2) click on the **DONE don't move label** button. With the first option, the label would be moved to a new position on the plot, which might be irritating if one had spent some time carefully positioning all the labels. With the second option, the curve characteristics are changed, but the label is returned to its old (previous) position.

Now move the mouse cursor over the Kaolinite label and click the left mouse button. Move the mouse cursor over the button labeled "no symbol" and click the left mouse button. The screen will appear as in Figure 4; a menu will drop down with numerous symbol options. Move the mouse cursor down over the star symbol as shown, and click the left mouse button.

Figure 4. Changing a curve symbol.

Try changing the Gibbsite and Muscovite curves on your own, by adding filled square symbols to the former and open circles to the latter.

once more appear as in figure 2.

button. The size of the Gibbsite label will change accordingly, and the menu bar will

size menu will drop down, as shown in figure 5. Click on one of the entries, then on the

cursor up to the top menu bar, then left-click on the light blue button labeled "Gibbsite". A text

Move the mouse cursor over the Gibbsite label and click the left mouse button, then move the

Figure 5. Changing the label text size.

From the main plot screen, select **File** by left-clicking with the mouse, or by pressing 'F' on the keyboard. The file menu will appear as in figure 6. Move the mouse cursor over the entry **Text font - Internal (simple)** and click the left mouse button, or simply type 'T' on the keyboard. The button will toggle from "Internal simple" to "External (TripleX)" as shown in figure 6. This step is not necessary to obtain output; it simply makes the plot prettier.

We may wish to print our finished plot, so we must select a graphics format. The current selection, **Graphics format - HPGL+LaserJet codes**, is good if we plan to print the plot to an HP LaserJet III or 4, directly from the DOS prompt. If we plan to import the graphic into WordPerfect for Windows, we should toggle the selection to read "HPGL WPWin 5.1/5.2", and if we plan to import into MS Word, we should toggle to "pure HPGL (MS Word)".

Click outside the file menu, or press the Esc key, to return to the main plot screen.

Figure 7. Setting a zoom box with the mouse.

Now move the mouse cursor above and to left of the Gibbsite label, click the **right** mouse button, and move the cursor down and to the right as shown in figure 7, sweeping out a zoom box. Click the **right** mouse button again to set the size of the box, then move the cursor inside the box and click the **right** button a third time to accept the box (clicking outside the box would abort the zoom). The region in the zoom box expands to fill the plot, as shown in figure 8.

Note that we did **not** use the Zoom button on the top menu bar. The Zoom button is provided for cursor-key-only zooming, and is aimed at lap-top or palm-top computers that lack a useful mouse. Similarly, the Label button on the menu bar allows rapid selection of labels without the use of a mouse, but has fewer editing capabilities than mouse-oriented editing.

Figure 8. The zoomed region.

Now restore the previous scaling by clicking on the **Back** button, or by pressing 'B' on the keyboard. Then return to the variables screen by clicking on the **Varia** button, or by typing 'V' on the keyboard.

In the plot so far, the mineral amounts are plotted against the **left vertical axis**. We now wish to plot the molalities of aluminum species, containing both Al and oxygen, against the **right vertical axis**.

Figure 9. Selecting Al-O species to plot on the right vertical axis. Note '&' can be used to separate word fragments.

First grab the slider of the scroll bar, and drag it down so it straddles the region between "SPEC" and "Q/K". To do so, position the mouse cursor over the bright blue slider on the right side of the screen, depress the left mouse button, and hold the button down while moving the slider to its new position, then release the mouse button. This step is not absolutely necessary, but makes it easier to see the changes.

Next click on the species icon with the **right** mouse button (or press shift-F3 on the keyboard). A dialog box comes up shown in figure 9, requesting word fragments for the search. Type in "Al & O", then click outside the dialog box or press the Enter key. Species containing both Al and O will be marked in the left-most column with an uppercase 'Y', indicating they are to be plotted against the right vertical axis.

Notice the **Keep y + x axes**, which shows PP's intentions to preserve the current x and y axis scaling. We could override this choice, and force PP to rescale the axes, by clicking 3 times on the button, until it reads "Keep nothing" (if you try that, click another 4 times to return to "Keep y + x axes" before proceeding).

Figure 11. Setting axis ranges with the Axes dialog.

Click the mouse on the **Axes** button (or press 'A' on the keyboard). Edit the entries as shown in figure 11: the left axis from -8 to 0, the right from -60 to -5, and the x axis from 0 to 0.00018. Then click on **F10= ACCEPT new values + exit.** (or press the F10 on the keyboard). Delete the curve for $\text{Al}_{13}\text{O}_4(\text{OH})_{24}^{+7}$, since this species has low concentration.

Send the plot to a graphics file by clicking on the **Output** button (or press 'O' on the keyboard). The screen updates slowly as PP writes each HPGL instruction to a default file named **hp.000** in the current directory.

Figure 12. PP graphics file **hp.000**, imported into WordPerfect.

PP produces HPGL (Hewlett-Packard Graphics Language) graphics files. Section 5.13 describes how to import these files into several popular applications, and how to print them directly to HP III and 4 laser printers. Figure 12, for example, was imported directly into this report with the WordPerfect 5.2 "Graphics-Figure-Retrieve" dialog.

We now consider a more complex plot, to illustrate the processes of importing data, editing labels, and searching the EQ3/6 database. The next example requires successive runs with the EQ6 input files **t4a.6i** and **t4b.6i** from the PP distribution. These input files were used to simulate the interaction of dissolving Calcite and Gypsum (run #1) and pure Calcite (run #2) with buried uranium oxide waste.

First create the **hwsdata** file by running EQ6:

```
runeq6 com t4a.6i ←
```

Then invoke PP, and click on the pH (in the top or "King" section), then click on the "ELEM" icon (or press F2) to mark these variables for export. Export the data by clicking on **Export** (or by typing 'E' on the keyboard). Press "Enter" (↵) on the keyboard to accept the default **txt.000** filename.

Figure 13. Selecting imported data.

Figure 13. Selecting imported data.

[illegible]

Next use the axes dialog to adjust the left axis to range from -12 to 2, and the right to range from 7 to 11, as shown in figure 15.

Some curve labels are duplicates, and others are not terribly descriptive. We wish to distinguish the curves that correspond to run #1 (the imported data, produced by the EQ6 run with $t_{4a}.61$) and run #2 (from $t_{4b}.61$), so it is necessary to edit the curve labels. Move the mouse cursor over the label "U mols" and double-click with the left mouse button. The edit dialog shown in figure 15 will appear. One can use the right and left arrow keys or the mouse to move about in the label. Edit the label to read "U #1", and press the Enter key. Repeat the process with the other labels, add symbols to the curves and change the line types, use the File dialog to change the font and number size on the axes, then click the **Output** button to produce a graphics file (if this is the second plot you have created with PP, the file name will probably be $hp.001$; see sections 5.9 and 5.12). Figure 16 shows the final plot, as imported into WordPerfect.

Figure 15. Editing a label.

Figure 16. Graphics file from figure 15, imported into WordPerfect.

Next we examine PP's ability to search the EQ3/6 database. Click on **Varia** to return to the variables menu, and drag the scroll bar slider about 1 cm below the red "Q/K" label to the right of the scroll bar, as shown on the right side of figure 17. Note the large number of Clinoptilolite entries; move the purple bar cursor over "Clinoptilolite-Ca" and type either '/' or '?' on the keyboard. The database search window will appear in the center of the screen with the corresponding entry in the EQ3/6 database. Typing 'R' at the keyboard will send the entry to both the printer and an appended file **thermo.txt**. Typing 'T' will switch to the "In CONTENTS" mode, which shows a compressed list of all the minerals and species in the EQ3/6 database used for the calculation, as shown in figure 18. One can scroll through these lists, examining data and even the references to the data, flipping between the "Text" and CONTENTS modes with the Enter key.


```

yxV
space PgDn, PgUp for more
CaAl2O4:10H2O      none Medium Medium pen1
CaAl4O7            none Medium Medium pen1
CaSO4:0.5H2O(beta) none Medium Medium pen1
CaUO4             none Medium Medium pen1
Gallite           none Medium Medium pen1
Carnallite
Print Esc Search: Clinoptilol Next Prev In-Text Back
Clinoptilolite-Ca  Ca1.7335Al3.45Fe+++0.017Si14.533036:10.922H2O
Chalcidate
date last revised = 26-jan-1990
Chamosite keys = solid idealized
Chloronite U0PrTr = 632.050 cm**3/mol (source = )
Chrysotile nut = 1344.41800 g/mol
Clinoch 6 chemical elements =
Clinoch 3.4500 Al 1.7335 Ca 0.0170 Fe
Clinopt 21.0440 H 46.9220 O 14.5330 Si
Clinopt 7 species in data0 reaction
Clinopt -1.0000 Clinoptilolite-Ca -13.0000 H+
Clinopt 0.0170 Fe+++ 1.7335 Ca++
Clinopt 3.4500 Al+++ 14.5330 SiO2(aq)
Clinopt 17.8560 H2O
Clinopt * log k grid (0-25-60-100/150-200-250-300 C) =
Clinopt -10.9121 -9.9581 -11.8090 -14.7647
Clinopt -18.2702 -21.3945 -24.3508 -27.4676
Clinopt * Extrapolation algorithm: cp integration
Clinopt * gflag = 1 (reported delG0f used)
Clinopt * basic source = 09db 7
Coesite * delG0f = -4547.700 kcal/mol
Coffinite none Medium Medium pen1
Colemanite none Medium Medium pen1
Cordierite anhyd none Medium Medium pen1
F1-Help Esc-exits Export Import PLOT Get put Keep nothing Files
F2-Elements F4-Minerals F6-log10(Q/K)
F3-Species F5-Cases F10-Clear all

```

Figure 17. Searching the EQ3/6 database.

yxV	L	M	S	T	C
space	PgDn, PgUp for more				
CaAl ₂ O ₄ ·10H ₂ O	none	Medium	Medium	pen1	
CaAl ₂ O ₄	none	Medium	Medium	pen1	
CaSO ₄ ·0.5H ₂ O(beta)	none	Medium	Medium	pen1	
CaUO ₄	none	Medium	Medium	pen1	
Calcite	none	Medium	Medium	pen1	
Carnallite	Print	Esc	Search: Clinoptilol	Next	Prev
Celadon	Clinoptilolite-Ca	Ca1.7335Al3.45Fe+++	017Si14.533036:10.922H2O	Im	CONTENTS
Chalcid	Clinoptilolite-Cs	Cs3.467Al3.45Fe+++	017Si14.533036:10.922H2O		
Chamosite	Clinoptilolite-K	K3.467Al3.45Fe+++	017Si14.533036:10.922H2O		
Chloran	Clinoptilolite-NH4	(NH4)3.467Al3.45Fe+++	017Si14.533036:10.922H2O		
Chrysot	Clinoptilolite-Na	Na3.467Al3.45Fe+++	017Si14.533036:10.922H2O		
Clinoch	Clinoptilolite-Sr	Sr1.7335Al3.45Fe+++	017Si14.533036:10.922H2O		
Clinoch	Clinoptilolite-dehy	Sr.036Mg.124Ca.761Mn.002Ba.062K.543Na.954Al3.45F			
Clinopt	Clinoptilolite-dehy-Ca	Ca1.7335Al3.45Fe+++	017Si14.533036		
Clinopt	Clinoptilolite-dehy-Cs	Cs3.467Al3.45Fe+++	017Si14.533036		
Clinopt	Clinoptilolite-dehy-K	K3.467Al3.45Fe+++	017Si14.533036		
Clinopt	Clinoptilolite-dehy-NH4	(NH4)3.467Al3.45Fe+++	017Si14.533036		
Clinopt	Clinoptilolite-dehy-Na	Na3.467Al3.45Fe+++	017Si14.533036		
Clinopt	Clinoptilolite-dehy-Sr	Sr1.7335Al3.45Fe+++	017Si14.533036		
Clinopt	Clinoptilolite-hy-Ca	Ca1.7335Al3.45Fe+++	017Si		
Clinopt	Clinoptilolite-hy-Cs	Cs3.467Al3.45Fe+++	017Si		
Clinopt	Clinoptilolite-hy-K	K3.467Al3.45Fe+++	017Si		
Clinopt	Clinoptilolite-hy-Na	Na3.467Al3.45Fe+++	017Si		
Clinopt	Clinoptilolite-hy-Sr	Sr1.7335Al3.45Fe+++	017Si		
Clinozo	Clinozoisite	Ca2Al3Si3O12(OH)			
Coesite	Cobalt	Co			
Coffinite		none	Medium	Medium	pen1
Colemanite		none	Medium	Medium	pen1
Cordierite anhyd		none	Medium	Medium	pen1
F1-Help	Esc exits	Export Import	PLOT	Get put	Keep nothing
F2-Elements	F4-Minerals	F6-log10(Q/K)			
F3-Species	F5-Cases	F10-Clear all			

Figure 18. CONTENTS mode for searching the EQ3/6 database.

Note that the EQ3/6 database can also be searched from the plot screen. To do so, left-click on the label of interest, move the mouse cursor onto the **What is this ???** button and click the mouse again.

The following four sections explain how to obtain help on-line, discuss the operations performed in the tutorial in greater detail, and explain how one edits the fonts and creates custom characters like those shown in figure 22.

3. Obtaining Help On-Line

Help is obtained by pressing the F1 key in the variables screen, in the plot screen, and in several sub-menus. The help window (figure 19) has three parts: 1) the main window, with a black background; 2) the Scrollbar on the right side, with a white slider that shows the current position in the help file; and 3) the menu bar at the top.

Figure 19. The help screen.

The main window displays either the text of the help file, or its table of contents. One can navigate through either by using the PgUp, PgDn and cursor keys. Alternatively, one can use the mouse to drag the slider on the scrollbar. To see the table of contents, type 'I', or click on "In Text".

The menu bar has 7 selections:

<i>F1=Help</i>	-- explains how to use the on-line help;
<i>Esc</i>	-- exits help;
<i>Search:</i>	-- allows one to enter search text for the "Next" and "Prev" commands;
<i>Next</i>	-- searches forward through the help file to find the next occurrence of the text entered via the "search" command;
<i>Prev</i>	-- searches backward to find the previous occurrence of the text;
<i>In ...</i>	-- indicates whether the main display is showing the CONTENTS, or the text of help file -- typing 'I' or clicking in the highlight bar toggles the mode;
<i>Back</i>	-- allows one to retrace steps, after using hot links to travel through the file.

One can choose a selection by clicking the left mouse button on the appropriate portion of the menu bar, or by typing the highlighted letter or key -- for example, typing 'S' brings up the search string editor.

When the "In" entry on the menu bar reads "CONTENTS", the help window displays a list of the main topics in the help file. There is a pink and green highlight bar across the screen, which can be moved up and down with the cursor keys or the mouse. Clicking on a contents selection with the mouse, or pressing the Enter key, moves to that entry in the help file.

3.1 Hot Links

When the "In" entry on the menu bar reads "Text", the main part of the window displays the text of the help file. Clicking the mouse pointer on a word or phrase that is highlighted in green causes the display to move to the associated topic in the help file. One can move repeatedly through the help file by following the hot links, then backtrack to the original position by clicking on the "Back" entry on the menu bar.

3.2 Searching

There are several ways to specify a search string. In both CONTENTS and text modes, one can type 'S' or click on the "Search:" highlight on the menu bar, then enter the desired search string at the prompt. In text mode (i.e., the right side of the menu bar reads "In Text"), one can click on any non-highlighted word to place it in the search buffer.

After a phrase has been entered in the search buffer, locate the next occurrence of that phrase by typing 'N' or '+', or by clicking on the "Next" highlight bar. Similarly, find the previous occurrence in the file by typing 'P' or '-' or clicking on "Prev".

3.3 Editing the Help File

The help file, **help_pp**, is mostly ASCII with a few pairs of formatting characters. To edit this file, use an ASCII editor such as DOS **edit** or the Windows **notepad**, and set the word-wrap on the 70th column. Unless one adds Hot Links or titles, it will generally not be necessary to add the formatting characters. The formatting characters consist of either ASCII 28 or ASCII 249 (PP regards the two as equivalent), followed by one of the letters u,U,d,D (for "up" and "down", used to sub or superscript text), x,X (to turn on xor mode), n,N (to turn off xor) or w,W, b,B, c,C, g,G, m,M, y,Y to turn on a particular color and brightness (white, blue, cyan, green, magenta, yellow, where capital letters denote bright colors). In DOS **edit**, ASCII 28 appears as a mid-line dot (•), and in **notepad** it may appear as an accented u (ù), depending on the active font. Both editors allow these characters to be replicated with the copy and paste commands.

There is one minor caution about editing **help_pp**. The help utility is entered through the C function **help(char *strng)**, which is mildly context sensitive, and finds its location in the help file by searching for the target "**strng**". Typically, "**strng**" refers to part of a section title in **help_pp**. Thus if section titles are arbitrarily changed, **help()** may not locate the appropriate section, and will simply default to the top of the help file.

4. The Variables Screen

The variables screen is divided into three horizontal regions, with pink (top of screen), white (middle), and dark cyan (bottom) backgrounds (figure 1).

The top (pink background) region lists what is in the columns of the middle region. The highlighted hot keys can be used to toggle through the choices in the columns. It is generally much easier to use the mouse to change the choices; just move the mouse cursor to the column and row to be changed, and click on the entry repeatedly to toggle through the choices.

The middle region displays the variables that can be plotted, along with their plotting attributes. The right side shows a scroll bar that represents the entire list of variables. The divisions between types of variables are marked on the scroll bar with dotted lines, and to the right there are abbreviations (e.g. "SPEC" for species) to indicate the types. The left and main part of this region is a "window" into the list of variables. The size of the window corresponds to the height of the slider (the slider is the light blue-green rectangle on the scroll bar). The scroll bar is the fastest way to navigate through the variables list; move the mouse pointer over the slider, then depress the left mouse button and hold it down while moving the slider to a new position. When the button is released, the left part of the screen will show the variables in this new region.

When the mouse pointer moves across the white region, a purple cursor bar follows along. The cursor bar can also be moved with the cursor keys (arrow keys), PgUp, and PgDn. We call the variable included in the cursor bar the "**current**" variable.

4.1 Selecting Variables (Variables Screen)

One can select variables to plot with the keyboard or mouse. Typing x, y, or Y causes the current variable to be selected as the horizontal, left vertical or right vertical axis, respectively. One can select any number of y or Y variables, but only one x variable for the original (non-imported) data, and one x for the block of imported data. Pressing the space bar, backspace or delete key erases the x, y or Y on the current variable.

To select variables with the mouse, move the mouse cursor over the variable name, then click the **left** button to select the variable as y (plots on left vertical axis), or the **right** button to select it as Y (right axis). If the mouse has a middle (third) button, clicking the middle button selects the current variable as x. A second click (with the same button) erases an entry. Note that as variables are selected, they are also marked as ticks to the left of the scroll bar, so it is possible to see a summary of all the selected data, even when the variables list contains tens of pages.

4.2 Plotting Attributes (Variables Screen)

The columns to the right of the variable name give the plotting attributes: the Line type used to connect the points on the plot, the type of Marker (marker=symbol, such as square or circle) plotted at each point, the Size of the marker, the size of the Text used for each curve label, and the Color ("pen") used to plot the lines, markers and labels. To change an attribute for a particular curve, move the mouse cursor over the column and row of the attribute, and click the left mouse button repeatedly to step through the choices. To make changes with the keyboard,

use the UP and DOWN arrow keys to position the cursor bar over the desired variable, then type the hot key (letter) corresponding to the column to be changed. The hot keys are shown at the top of each column, and are highlighted in bright white on a dark green background:

For example, type 'L' repeatedly to toggle through the line type choices for that variable. All these attributes can be edited in the plot screen as well (perhaps much more intuitively), so it is not necessary to get all the selections exact.

4.3 Icons and Variable Groups (Variables Screen)

To the right of the attributes are some simple icons, denoting the following groups of variables:

- KING* -- a yellow crown, denotes what are sometimes called "master" variables, such as pH, Eh, reaction progress and time;
- ELEM* -- blue waves, denotes the bulk elemental composition of the aqueous phase in moles;
- MIN* -- a reddish octahedron, denotes the amounts of minerals present in the system, in moles;
- SPEC* -- waves with + and - signs dispersed throughout, denotes the molalities of dissolved species in the aqueous phase;
- Q/K* -- a ghosted ("dissolving") octahedron, denoting the saturation state of all possible minerals or solid phases;
- GAS* -- a cloud to denote gas fugacities;
- IMPO* -- a distinctive icon, present only when data are imported.

The icons are placed at the top of each group of variables. The variable groups are further distinguished by alternating gray or black text for the variable names, and dashed line separators at the start of each group.

Clicking on the ELEM, MIN, Q/K, GAS or IMPO icons selects some subset for plotting. Clicking with the left button selects the variables for the left axis (y); the right button selects them for the right axis (Y). Clicking on the ELEM icon selects all elements but hydrogen and oxygen; clicking on the MIN icon selects all minerals; clicking on Q/K selects all minerals with saturation states above 0.001; clicking on the IMPO icon selects the first imported variable as x, and the rest as y or Y. Clicking on SPEC (species), however, brings up a search dialogue. All species names containing the entered substrings will be selected for plotting. One can select species based on more than one word fragment. For example, to find all species with both Ca

and O, one would type "Ca & O" at the prompt (without the quotes).

4.4 Buttons (Bottom of Variables Screen)

The bottom of the variables screen contains light cyan "buttons" with red highlights:

The button functions can be activated by clicking on the buttons with the mouse cursor, or by typing the red-and-white-highlighted key. The F1 button brings up the help screen (figure 19), and Esc exits the program. The F2 through F6 buttons mark subsets of the variables as indicated above, and duplicate the purposes of the icons, principally for use with lap-top computers. To mark y vs. Y subsets, one can click the left or right mouse buttons, respectively, or type the function key alone for y, and shift-function key to select Y. The F10 key clears (deselects) all the y variables, and shift-F10 clears all the Y variables. Actions performed by the remaining buttons are slightly more complicated and are discussed in detail below.

4.5 The PLOT Button and Sorting (Variables Screen)

There are three ways to plot the selected data (and thus leave the variables screen). First, one can click on the PLOT bar at the bottom of the menu; second, just type 'p'. Third, typing 'control p' (that is, holding down the control key while pressing 'p') sorts the x axis before plotting.

How is the 'control p' option different? Normally, PP plots the x,y and x,Y pairs in the order they were created by the reaction path program. Sometimes the result can be a little disconcerting; in a plot of aqueous composition vs. pH for example, the curves may wrap back on themselves, since pH may rise and fall in a calculation. By using the 'control p' option, the x data will be sorted to avoid the wrap-back.

4.6 Templates: Saving (pUt) and Retrieving (Get) Plotting Attributes (Variables Screen and Plot Screen)

Often successive reaction path calculations use very similar conditions, and it is desirable to plot the results of each calculation with the same axis ranges, same symbols and line type, *etc.* The "pUt" command (in both the variables and plot screens) makes it possible to save templates that preserve the axis ranges, symbol types and sizes, font, text size, *etc.* Typing 'U' or clicking on the pUt button brings up a dialog box requesting a template name, with a default of **template.tmp**. The "Get" command (type 'G' or click on Get) performs the inverse, retrieving a template, again with the default name **template.tmp**.

The template files are ASCII, and can be edited, but do so at your own risk, since the order of data in the templates is important.

4.7 Exporting Data (Variables Screen)

The "Export" button at the bottom of the screen saves the data marked with x,y or Y to a tab-delimited ASCII (text) file. This type of file can be read, transparently, by many spreadsheet

and graphics programs. In the ASCII file, each column will represent a variable. The first row of the column will be the variable name, and the following rows will be the values of the variable at successive steps in the calculation.

Clicking on Export (or typing 'E' at the keyboard) brings up a dialog box requesting a file name; pressing the return key or clicking outside the box accepts the default file name (initially **txt.000**). PP autoincrements export file names, so the next default name would be **txt.001**, etc.

4.8 Importing Data (Variables Screen)

The "Import" button performs the inverse of Export. Clicking on Import (or typing 'I') brings up a dialog box with the default file name **txt.000**. PP expects the import data to be in columns of equal length, and the first entry of each column is assumed to be the curve label (if the columns are of unequal length, pad them with repeats of the last real datum). Spaces, commas, and tabs may be used as delimiters, and MUST NOT appear in the labels or data entries. If it is necessary to indicate spaces in a label, use underscores, which PP will convert into spaces. Here is an example of a valid import file:

```
wombat_ears pH pickle_#
0.05  1.0  1e-7
0.1    2.0  1.2e-7
.13    2.5  1.3e-7
.17    3.0  3e-7
.25    3.3  1e-6
.36    3.45 1e-5
.56    3.6  1e-4
.7     3.6  1e-4
.9     3.6  1e-4
.99    3.6  1e-4
```

The formatting requirements are not very strict. The columns can have varied numbers of spaces separating entries, and do not need to be aligned. The labels need not have any connection to the variables in EQ6.

If the data are imported successfully, PP will place them at the end of the variables screen in a section called "IMPO", with a distinctive icon. In the example above, PP would replace the underscores with spaces, creating variable names "wombat ears" and "pickle #".

The main purposes of the import function are:

- (1) to allow results of successive reaction path runs to be merged and viewed together;
- (2) to superpose experimental results or literature values on the plot.

The tutorial contains an example of case (1) (figures 13 - 16).

The imported data are regarded as "guests", and cannot be plotted by themselves; at least one "host" x,y or x,Y pair must be selected from the other (non-imported) data. One can select one x and many y or Y variables in the imported section. If no x variable is selected, the imported data will not appear on the plot. Remember that step sizes in reaction path calculations vary from run to run, so don't expect the nodes of the curves to line up with the results of the current run.

4.9 The Keep Button (Variables Screen)

Note the "Keep" selection in the bottom part of the variables screen. Each time the user moves between the variables and plot screens, PP tries to guess if it should keep (preserve) the plot axis ranges and the label positions, or automatically rescale to accommodate new data selected in the variables screen. In effect, PP tries to save all the labor expended zooming the plot or moving labels. The "keep" button displays the current state of affairs, as judged by PP.

In most cases the user can ignore the Keep button, and accept PP's decisions about rescaling. However, PP's choices can be overridden. Clicking on the Keep button toggles through the following choices:

- (1) *Keep nothing* - the next plot will rescale all axes and reposition labels near the curve maxima;
- (2) *Keep left y axis* - the next plot will preserve the scaling on the left y axis, but rescale x and Y (right vertical axis) and move labels ;
- (3) *Keep right Y ax.* - the next plot will preserve the scaling on the right Y axis, but rescale x and y (left vertical axis) and move labels;
- (4) *Keep y + Y axes* - the next plot will preserve the scaling on the left y and right Y axes, but rescale x and move labels;
- (5) *Keep y + x axes* - the next plot will preserve the scaling on the left y and x axes, and rescale the right Y; label positions associated with the left axis will be preserved;
- (6) *Keep Y + x axes* - the next plot will preserve the scaling on the right Y and x axes, and rescale the left y; label positions associated with the right axis will be preserved;
- (7) *Keep all axes* - the next plot will preserve the scaling on all axes, and preserve all label positions.

Note that subsequent actions in the variables screen may still override a manual Keep selection. Suppose, for example, the user selected "Reaction progress" as the x variable for the plot, then toggled "keep" to selection (5) above (Keep y + x axes). If the user subsequently changed the x variable from "Reaction progress" to "pH", PP would downgrade the "keep" selection to (2) (Keep left y axis).

The "keep" option is a mixed blessing; a user returning to the variables menu probably plans to

add another curve, which may be way off scale if the axes are not rescaled automatically. If an expected curve seems to have vanished, try toggling the Ylin/LOG and ylin/LOG buttons on the plot screen, or return to the variables menu and toggle "Keep" to "Keep nothing" to force a rescaling.

4.10 The mOles / MOLAL Button (Variables Screen)

This button affects only the ELEM data (bulk composition of the aqueous phase), and toggles the plotting units between total moles and molal.

By default, data in the ELEM section are given in moles. Since EQ3/6 defaults to 1 kg. of H₂O for calculations, these data will often correspond to molality. However, in reaction paths that involve evaporation, it may be more appropriate to plot the molality of each element dissolved in the aqueous phase. In the future, a "ppm" (parts per million) option may be added as well.

5. The Plot Screen

Selecting "PLOT" at the bottom of the variables screen brings up the plot screen. The program tries to pick reasonable axis ranges, and attempts to pick pleasing subdivisions for tick marks. The curve labels (e.g., $\text{Al}_2(\text{OH})_2^{+4}$) are placed near the highest position on the curves, and at this stage may overlap. However, it is easy to adjust the default scaling and labels.

The top of the plot screen contains a row of 14 buttons:

F1=Help Esc=Quit Varia File Axes Output xlin yLOG yLOG Label Zoom Back Get pUt

The buttons are activated by clicking on them with the mouse, or by pressing the key indicated by the red and white highlight. Below is a quick summary of the options available in the plot screen, as they are listed on the menu bar at the top of the screen:

- F1* -- brings up the help screen;
- Esc* -- leaves the program (there is a chance to cancel);
- Varia* -- returns to the Variables screen;
- File* -- brings up a menu for changing output file characteristics, including
 - output file name,
 - graphics format (pure HPGL vs. embedded printer codes),
 - font (default vs. Roman-like triplex),
 - use of Minor ticks,
 - size of numbers on axes,
 - pen width,
 - arrow size and type;
- Axes* -- brings up a dialog for changing axes ranges (see 5.2 "Zooming with the Mouse");
- Output* -- sends the plot to a file or hardcopy device ("prints" the plot);
- x,y,Y* -- toggle the x,y,Y axes between LOG and linear display;
- Label* -- adjusts label positions by keyboard (see 5.3 Changing Curve labels);
- Zoom* -- zoom part of the plot by keyboard (see also 5.2 Zooming with the Mouse);
- Back* -- undoes the last zoom;
- Get* -- get (retrieve) plot Templates, i.e. stored axis ranges, variable selections; symbol (marker) and line types (same as variables screen Get);
- pUt* -- put (save) a template to a file for later reuse (same as variables screen pUt).

5.1 Changing Axes Ranges and Scaling (Plot Screen)

First off, the default choice of log vs. linear scaling may be inappropriate. For example, pH should be plotted on a linear, rather than $\log_{10}$ scale. The defaults can be changed with the x, y, and Y toggles at the top of the screen, which affect the corresponding horizontal, left vertical and right vertical axes.

The axes ranges can be altered in several ways. If exact limits are desired, it is best to use the axes dialog (type 'A' or click on the "Axes" button at the screen top; figure 11), which allows one to type in the desired ranges. If exact ranges are not needed, it is often faster and more intuitive to zoom with the mouse.

5.2 Zooming with the Mouse (Plot Screen)

To zoom with the mouse (figures 7 and 8), move the mouse to one corner of the desired zoom area, click the **right** button, then move the mouse till the zoom box is the desired shape (if a mistake is made, type Esc to exit). Then click the **right** button once more to fix the shape of the zoom box. Clicking the **right** button once more INSIDE the zoom box rescales the plot to make the zoom box full screen. If one types Esc or clicks outside the box, the zoom will abort. To return to the previous scaling, click on the "Back" button on the top right side of the screen.

Note that before the final click is made inside the zoom box, there is an option to print the plot with the zoom area indicated as a dashed box. Just press the "O" key to create an output file with the dashed box, then click inside the zoom box to finish the zoom.

5.3 Changing Curve Labels, Markers (Symbols) and Line Types (Plot Screen)

The simplest way to move or edit the labels and change the curve symbols, curve color, line type, and label size is with the mouse (figures 3-5).

To *edit* a curve label, double-click on the label with the **left** mouse button. An edit dialog box will then pop up. Pressing the return key or clicking outside the box accepts the new label. To "double-click", press the button twice in rapid succession. The double-click delay is ≈ 0.35 seconds, which is comfortable for most users.

To *move* a label or change the curve characteristics, single-click on the label with the **left** mouse button. The label is then "attached" to the mouse cursor, and can be moved to another position (it is NOT necessary to hold down the mouse button to "drag" the label). Typing 'A' will draw an arrow to the nearest node on the curve; typing 'E' will erase an existing arrow (see section 5.8 for the method of changing the arrow type). Clicking another mouse button in the main part of the screen fixes the label in that new position.

Single-clicking on a label places a new menu at the top of the screen, displaying seven buttons, six of which are light cyan (light blue-green):

The left-most selection on the menu deletes the curve and label, providing a means to clean up a complex plot. The next button to the right allows one to change the line type used to connect the curves; clicking on this selection brings up a menu with available line types. Similarly, the next selection to the right allows one to change the size and type of symbol used on each plot point (figure 4). The next allows the user to select one of four text sizes for the label (figure 5), and the next selection makes it possible to change the color of the curve, symbols and text. The sixth button searches the EQ3/6 database for the thermodynamic and composition data of the label, so the user who has forgotten the composition of "Boehmite" can get a refresher (see section 1.2 "Installing PP" to make sure the search path is set correctly, and section 5.4 "Searching the EQ3/6 Database" for more detailed discussion). This menu reduces the need to return to the variables screen.

5.4 Searching the EQ3/6 Database (Plot Screen and Variables Screen)

From both the variables screen and the plot screen, one can obtain composition and thermodynamic information about the minerals and species in the variables list. In the variables menu, move the cursor over the variable of interest, then press either '/' or '?'. A screen similar to the help screen will come up with the corresponding entry in the EQ3/6 database (figures 17-18). There may be a delay of a second or so -- the databases are often several megabytes in size. One can then search through the database for any other species of interest; pressing the 'I' key toggles to a listing of all the available species data used by EQ3/6. If PP cannot find the database, it will display an error message; in such case, be sure the environment variables set correctly (see section 1.2, "Installing PP").

To search the database from the plot screen, right-click the mouse on the label of interest, then either choose the "What is this ???" button on the top right side of the screen, or type '/' or '?' at the keyboard (see also section 5.3 "Changing Curve Labels").

5.5 Changing Axis Labels (Plot Screen)

To change the axes (axis) labels, click over the label with the left mouse button. A dialog box will pop up with the current name. Pressing "Enter" or clicking outside the box uses the new value.

5.6 Templates (Get and pUt) (Plot Screen)

Templates can be saved and retrieved from the plot screen. See the discussion of Templates in section 4.6.

5.7 The Zoom and Label Buttons (Plot Screen)

The "Zoom" and "Label" selections on the menu bar provide for keyboard-only editing on lap-top computers that lack a mouse or other useful pointing device. Each option contains two extensive submenus to describe each process. The mouse zoom and label operations are generally much simpler and allow more editing options. However, the keyboard-only process for moving labels has one distinct advantage; the curves and labels are selected by scrolling through the list with the up and down arrow keys, eliminating the need to "hunt and peck" for labels in a complex plot.

5.8 File Options: Output File Characteristics, Plot Appearance (Plot Screen)

Clicking on the "File" button (or typing 'F') in the plot screen brings up a menu with the following options (figure 6):

<i>Esc</i>	-- clicking on this button leaves the File menu;
<i>output Filename=</i>	-- allows one to change/edit the output filename;
<i>Graphics format=</i>	-- toggles among "HPGL+laserjet codes", "pure HPGL (MS Word)", "HPGL WpWin 5.1/5.2";
<i>Text font=</i>	-- toggles between "Internal (simple)" and "External (Triplex)";
<i>use Minor ticks=</i>	-- toggles between "Yes" and "No";
<i>number Size=</i>	-- toggles among small, Medium, *BIG* and HUGE! for the size of the numbers on the x, y and Y axes;
<i>pen Width (mm)=</i>	-- selects the width of the plotter "pen" for HPGL files (affects hardcopy, not screen appearance);
<i>Arrow type=</i>	-- toggles among thin lines (no arrow head), and thin, Medium and FAT arrows with heads (figure 4);
<i>print QA banner=</i>	-- toggles between "NO" and "Yes"; the latter places a distinctive banner in the upper left corner of plots, to aid traceability.

The significance of several of these options is discussed in detail below.

5.9 Changing the Output File Name (Plot Screen, File Submenu)

The default output file names are **hp.000**, **hp.001**, **hp.002**, *etc.* The name can be changed with the "File" option on the main menu bar. PP automatically increments most file names, starting with the extension. Thus if one chooses a file name of **myfile.000**, the first "Output" file will indeed be called **myfile.000**, but the subsequent times one clicks on "Output", the files will be named **myfile.001**, **myfile.002**, *etc.* If one were to chose a file name of **dog**, subsequent names would be **doh**, **doi**, **doj**, ... **dpa**, **dpb**, ... *etc.* See section 5.12 for information on how PP preserves file names between sessions.

If file the name is **prn**, **lpt1**, or **com1** to **com4**, the file will be sent to the hardcopy device (printer or plotter) on that port. If the file is sent directly to a hardcopy device, be sure the device is in HPGL mode, or choose "HPGL+laserjet codes" format in the File Options menu.

5.10 Changing the Text Font (Plot Screen, File Submenu)

PP has two fonts -- a simple "internal" font, and a more complex, roman-like "external" or "triplex" font. To change the font, go to the Plot screen and type 'F' or click on 'File' (File Options) to bring up the submenu for graphics file options. Then type 'T' or click on "Text font" to toggle between the two choices. The external (triplex) font may look better, but it can make the HPGL file 3 times larger, and takes longer to print.

To use the external font, PP must be able to find the file **external.fnt**. To make sure PP finds this file, either place it in a directory called **\pp**, or the current working directory, or set the PP environment variable to point to the directory where the font is stored.

The internal font is compiled into pp.exe, and can not be changed. However, given patience it is possible to create a new external font with the program **ff.exe**. The later program can also be used to create custom symbols (markers), and is described in section 6.

5.11 The QA (Quality Assurance) Banner (Plot Screen, File Submenu)

Selecting "Yes" places a banner in the upper left corner of the plot, *e.g.*:

```
PWD=C:\PP OF=hp.004 DB=data0.com.R22a MachineID=1528 08-17-94 12:12
|EQ6 input file name= micro.6i BIN=hwsdata PPVER=1.01
```

The first line of the banner contains 6 entries. "PWD=" gives the present working directory, where PP was invoked. "OF=" is the name of the output file. "DB=" gives the name of the database used in the EQ3/6 run, along with its version number. "MachineID" gives the sum of the first 4096 bytes of the PC BIOS at **0xfe000** (each byte is converted to an unsigned 32-bit integer before summing). Since machine BIOSes usually have dates and serial numbers, it is extremely likely that this number will uniquely identify the machine used for the plot. The last two entries on the first line give the date and time of the plot.

The second line of the banner has three items. The first item is the first line of the EQ6 input file (not including the "I-----" line for the EQ6 "D" format). It is customary to place the input file name on the first line of an EQ6 input file, providing traceability. The second item, "BIN=" is the name of the binary plot file read by PP. The third, "PPVER=" gives the PP version number.

5.12 The Preferences File (prefer.pp)

When PP terminates, it saves all the selections in the File Submenu to a binary file called **prefer.pp**. The next time PP is invoked, it searches the working directory for this file. If **prefer.pp** is found, PP reads in the preferences, including the next name for the graphics output file. Thus if one prefers to always use the triplex font, one should not have to go to the File menu every time PP is invoked to make this selection. This process takes place transparently. Since PP only searches the local directory for **prefer.pp**, a separate copy can be kept in each subdirectory, reflecting different preferences for different sets of reaction path

runs. Deleting this file returns the File Submenu to its defaults.

Note that the "next" graphics output filename is stored in **prefer.pp**. Thus if one invokes PP and saves files **hp.000** and **hp.001**, quits the program, and starts it again two days later in the same directory, the next saved file will be called **hp.002**. The autoincrement process would continue through file **hp.999**, then would wrap back to file **hp.000**.

5.13 Output -- Printing, Hardcopy, Importing Plots into Word Processors (Plot Screen)

Use the "Output" button (or type 'O') to send the plot to a file. Currently, PP produces only HPGL (Hewlett-Packard Graphics Language) files. However, future versions of the code may support PostScript. HPGL files are understood by most PC-based applications, and can be imported into most CAD programs and all versions of WordPerfect ≥ 5.0 .

There are three ways to obtain hardcopy plots:

- (1) Send output directly to a plotter or printer from within PP;
- (2) Create plot files with the Output button, quit PP, then print the plot files from the DOS prompt;
- (3) quit PP and import the plot files (*e.g.* **hp.000**, **hp.001**) into a word processor or CAD program.

The first method works with an HP Laserjet III or 4 printer, a compatible laser or inkjet printer with an HPGL emulation mode, or a true HP plotter (7400 series or later). Use the File dialog (section 5.8) to select "Graphics format= HPGL + laserjet codes", and set the "output Filename" to be PRN or the port appropriate for your hardcopy device (*e.g.* LPT1, COM1, COM2). Leave the File dialog and click on the Output button; the screen will update slowly as the individual HPGL commands are written to the device. In rare circumstances, the printer may "time out" while the file is being printed, but the timeout should be intercepted by PP's critical error handler.

The second method works with the same devices as the first method. At the DOS prompt, one types **print hp.000** ← to print the file **hp.000**. The "Graphics format= HPGL + laserjet codes" selection creates files that contain the codes necessary to put most HP-compatible printers into plotter mode, as well as the codes to put the printer back in PCL mode and eject the page at the completion of the plot. These codes are on the very first and very last lines of the file, are preceded by ASCII 27 (the escape character, a left-pointing arrow), and can be removed with an ASCII editor.

The third method requires one to "import" the file into a program, such as a word processor. This method is the most flexible, since word processors and CAD programs have drivers for virtually all plotters and printers, and one can often edit or annotate the plot with the program.

For WordPerfect for Windows, best results are obtained when one chooses the "HPGL WpWin 5.1/5.2" format from the File dialog. In version 5.2, the "Graphics-Figure-Retrieve" dialog is then used to import the file. Files created with the "HPGL+laserjet codes" and "pure HPGL (MS Word)" options can still be imported, but it is best to first convert them to ***.wpg** files with the "Graphcnv" utility, using the /w switch to ensure thin

lines, *e.g.*:

```
\wpc\graphcnv hp.000 hp.wpg /w
```

To produce HPGL files for MS Word, use the "pure HPGL (MS Word)" format in the "File options" menu. However, one can import a file produced with the "HPGL+laserjet codes" option by first editing the "SC command" in the output file. This command will be on the 1st or 2nd line, and will be similar to:

```
IN;RO90;IP;IW;SC0,7990,0,5990;FT1;PA;SP1;
```

the 7990 and 5990 refer to the maximum x and y coordinates for the plot (these numbers might be different on your system) . To have MS Word import the plot, increase these numbers by a factor of about 1.25 -- *e.g.*, increase 7990 to 9980, and 5990 to 7480. If the increase is not made, the MS Word import filter will chop off the right and upper margins. Remember that these changes should be unnecessary if the "pure HPGL (MS Word)" option is chosen from the file menu in the plot screen.

To import an HPGL file in MS Word for Windows, one typically selects "insert" from the top menu bar, then "picture", then one uses the file dialog to select the file name. Once the picture is imported, double-clicking on it will bring up a picture editor that allows one to add text, draw lines, *etc.* on the figure. This picture editor is called MS Draw; while it comes with Word, it may not be installed on all systems.

If MS Word cannot read the HPGL files, it may be necessary to install the MS graphics filters. These filters are independent of MS Draw, and many system administrators DO NOT install them by default. With MS Word for Windows, the filter installation is performed *via* the setup program (typically on the installation floppy disc). Choose the custom installation, and unselect every choice except installation of the graphics filters, then click on the filters button and unselect every filter except the HPGL filter. To "unselect" an option, click on it with the mouse to remove the cross from the selection box.

Some applications may require that the HPGL files be converted into PostScript. In such a case, the public domain conversion program **hp2xx** (widely available on internet) can be used to make the conversion. For example, the DOS version could be used to convert the HPGL file **hp.000** to an encapsulated PostScript file **out.ps** *via*:

```
hp2xxdos -m eps -f out.ps hp.000
```

out.ps can then be imported into a word processor and embedded in a document.

6. The FF Font Editor

The program **ff.exe** can be used to edit PP's "external" font (figure 20). Copy the file **external.fnt** to **external.bak** and **test.fnt**, then start FF. In FF, click on "Retrieve" (or type 'R') to edit **test.fnt**. The screen will display an exclamation point, '!', which is ASCII character number 33, the first printable character. Clicking repeatedly on the "Next" button (or typing 'N') will advance through the successive ASCII characters:

" # \$ % & ' () * + , - . / 0 1 2 3 4 5 6 7 8 9 : ; < = > ? @ A
B C D E F G and so on.

To create a new character, or add a line to a character, move the mouse cursor to the desired position and click the **left** mouse button. A green "rubber band line" forms, with one end attached to the position of the last **left** click, and the other attached to the mouse cursor; the program is now in drawing mode. Each subsequent **left** click tacks down the "rubber band" to that position on the screen. If you make a mistake, press the *Escape* key to detach the last point; pressing *Escape* repeatedly will eventually "erase" the line. To complete the line, and leave drawing mode, click the **right** mouse button. The completed line turns from green to yellow. Each character may have up to 32 polylines, each with up to 32 x,y pairs (or 31 line segments per polyline).

To edit an existing line, move the mouse cursor near the line and click the **right** mouse button. The mouse cursor will attach itself to the end of the nearest line; the line can be deleted by repeatedly pressing the *Escape* key. The program will remain in drawing mode until one either deletes all the points on the line, or clicks the **right** mouse button.

Note the light cyan buttons on the right side of the screen. The "Quit" button exits the program. Clicking on the "Grid" button toggles the display of the positioning grid on and off. Toggling the "snAp" button ON forces the mouse pointer to move in 8 pixel increments on the grid. The "Retrieve" button pulls in the file **test.fnt** for editing; the "Save" button saves the same file. "Next" and "Previous" move forward and backward in the ASCII character set (the corresponding ASCII character is displayed at the bottom of the screen). The "Zero line" button allows one to change the position of the y-axis zero line. The default position is at the bottom of the screen, but the zero line should be moved up for characters with descenders, such as y,p,g, and j.

When done editing, be sure to save the altered file (by clicking on "Save" or typing 'S'), exit FF (by clicking on "Quit" or typing 'Q'), and copy **test.fnt** to **external.fnt**.

The FF editor can also create custom symbols (markers) to plot at the nodes of the reaction path curves (figure 21). The eight characters from ASCII 128 to 135 in **external.fnt** are reserved for custom symbols (in the standard PC character set, these are the letters Ç,ü,é,â,ä,å, and ç). When invoked, PP scans these characters to see if they have been defined (that is, if they contain any lines). If defined, the custom symbols are added to the selections available from the variables and plot screens.

Custom symbols should be drawn in FF so they nearly fill the width of the grid. The symbols will look best if they are roughly "equant" -- that is, not much taller than they are wide. And most important, the zero line should be set across the middle of the symbol, else the symbols will not be centered on the final plots.

Figure 20. Using FF to edit the letter 'Q'. A right mouse click has selected the nearest polyline for editing.

Figure 21. Using FF to edit a custom symbol in the font file (**external.fnt**).

There are two significant differences between custom symbols and the ordinary symbols (such as circles and squares) built into PP. First of all, the custom symbols plot larger; it is assumed that the larger size will be needed to show the details of the symbol design (figure 22). Second, PP generally does not draw lines through the custom symbols, since the lines would obscure the details. However, connecting lines are plotted between the symbols wherever possible.

Figure 22. Using custom symbols in a plot.

7. Implementation Details

PP is written in C, and compiled with Symantec C version 6.0, using the `-4 -mx -f` switches and no optimization. With comments, there are approximately 10000 lines of source code. The screen graphics primitives, such as line-drawing, pixel plotting, bitblt, and character printing, are provided by the FlashTek "Flash Graphics" libraries. The executable contains a DOS extender, so that when the program is invoked from the DOS prompt, the CPU is placed in protected mode with a 32-bit, flat address space.

Nearly all of PP's arrays are allocated dynamically. Thus, PP will adjust its memory requirements to the number of variables used by the EQ6 run that produces the **hwsdata** file. When data are imported, many of the arrays are reallocated to provide consistency in the graphics routines. The functions that display the **help_pp** and **data0.*** files read and allocate memory for these files with each invocation, and deallocate the memory at the completion of the function call. Thus each help or search call must re-read the files from disk; this process may seem inefficient, but allows PP to run on minimal systems, and in practice the delays are small.

The PP source code uses EQ6 notation for arrays whenever possible. For example, the PP array of mineral names is UMIN, and the array of "moles of total elements in aqueous solution" is called MTEAQ. However, if an EQ6 data array (as opposed to name array) has dimension N, the corresponding PP array generally has dimension N+1, where the extra dimension is the step number. The PP data arrays are declared as, *e.g.*,

```
double **MTEAQ.
```

PP contains numerous algorithms for editing text lines, drawing stroked fonts, parsing species formulae, clipping, and choosing axis ranges and increments. The editing, font, parsing and axis algorithms were developed independently by the author. The clipping functions are substantially modified versions of the NCSA Telnet routines. The NCSA routines are not copyrighted and are derived from the Liang-Barsky algorithm (Liang and Barsky, 1984). The NCSA code follows the published algorithm, maintaining the same variable names and changing only from Pascal to C syntax. We gratefully acknowledge the generosity of NCSA in making these routines available.

Currently, the most serious shortcoming of PP is the slowness of the text operations. Overall, the FlashTek graphics routines are very good. However, the FlashTek text routines preserve the background behind each character; this feature is quite ingenious, but is undesirable for PP and adds enormous overhead. It is estimated that the FlashTek bit-mapped text graphics are approximately 20 times slower than the equivalent MS Windows routines for modern, accelerator-based graphics cards. This slowness is manifest in high resolution modes (1024 by 768 pixels or more), where it may take a second to paint the screen on an ISA-bus 486 computer. In addition, many of the Symantec string functions are C compiled for the 386, and could be greatly improved by translation to assembly language, or recompilation for the Pentium.

8. Conclusions

PP provides a simple but flexible interface to EQ6, allowing rapid analysis of reaction path runs. Simple plots of one data type (*e.g.*, mineral amounts or solution composition) require two mouse clicks -- one to select the data, and one to plot. The program is designed for rapid navigation through the variable list, with a minimal amount of detail to confuse the user. While the user is free to select and customize axis ranges, most scaling decisions take place transparently, without user intervention. PP accommodates the specialized needs of reaction path plots, and simplifies the process of placing and editing labels and curve characteristics. Compatibility with other DOS and Windows programs is provided by a simple, standardized graphics format (HPGL), and the ability to export and import spreadsheet and ASCII data files. Useful changes for future versions of PP would include: improved speed of text operations; and migration to a richer operating system, such as MS Windows.

9. References

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- Liang, Y.-D. and Barsky, B.A. (1984) A new concept and method for line clipping, *ACM Transactions on Graphics* v **3**, pp 1-22.
- Wolery, T.J. (1992) *EQ3/6, A Software Package for Geochemical Modeling of Aqueous Systems: Package Overview and Installation Guide (Version 7.0)*. UCRL-MA-110662 PT1, Lawrence Livermore National Laboratory, Livermore, CA 94551, 66 pp.

10. Definitions, Copyrights and Trademarks

386, 486DX, 486SL	32-bit Microprocessors, trademarks of Intel Corporation
ASCII	American Standard Code for Information Interchange
BIOS	Basic Input-Output System, a series of machine-code programs for communicating with disk drives and peripherals, located in read-only memory (ROM)
bitblt	A block move of pixels
DOS	Disk Operating System
EQ3/6, EQ6	Equilibrium/reaction path codes copyrighted by University of California
FlashTek	Trademark of FlashTek, Inc.
Hewlett-Packard: laserjet, 1200C, 7400 series	Trademarks of Hewlett-Packard Corp.
HPGL	Hewlett-Packard Graphics Language, a vector plotter language
IBM	Trademark of International Business Machines Corp.
MB	Megabyte, or 2^{20} 8-bit bytes
Microsoft: MS DOS MS Draw MS Word notepad	Trademarks of Microsoft, Inc.
NCSA	National Center for Supercomputing Advances
PCL	Printer Command Language (Hewlett-Packard)
Pentium	32/64-bit microprocessor, trademark/copyright of Intel Corp.
pixel	A single (x,y) addressable point on a graphics screen
PostScript	A page-description language, trademark of Adobe Corp.
RAM	Random Access Memory (electronic memory)
reaction path	A record of the molar amounts and activities of species and components in the aqueous, solid and gaseous phases of a chemical system, as components are incrementally added or removed.
ROM	Read-Only Memory (electronic memory)
Symantec	Trademark of Symantec Corp.
VESA	Video Electronics Standards Association
VGA	Video Graphics Array, trademark of IBM Corp.
Windows	Trademark of Microsoft, Inc.
WordPerfect	Trademark of WordPerfect Corp.

APPENDIX: EQ6 Modifications for Creating HWSDATA

PP reads binary data files created by a modified version of EQ6. EQ6 was written by Thomas J. Wolery of Lawrence Livermore National Laboratory (LLNL), and is copyrighted by that author for the Department of Energy and the Regents of the University of California. The process for obtaining the EQ6 source is described in the EQ3/6 documentation (Wolery, 1992). This appendix describes the changes one must make to EQ6 to produce the **hwsdata** binary file, but does not contain any EQ6 code. It is assumed that EQ6 will subsequently be recompiled with Lahey FORTRAN or a compatible compiler.

The following function should be appended to the EQ6 source:

```

c=====
      subroutine hws4io(kstep, xxi, xxlkeh, nnhydr)
      implicit logical(q), integer(i, j, k, n), real*8(a-h, l, m, o, p, r-t, v-z),
      $ character*8(u)
c-----
c INSERT standard EQ6 parameter statements here, from ntitpa to nsspar
c-----
c INSERT the following EQ6 include files here:
c eq6af.h eq6dd.h eq6dzi.h eq6ff.h eq6gg.h eq6hh.h eq6ka.h
c eq6lm.h eq6mt.h eq6mta.h eq6ni.h eq6qq.h eq6rc.h eq6re.h
c eqlpp.h eq6ki.h eq6si.h eq6ti.h
c-----
      dimension ihws(nmtpar)
      dimension ihit(nmtpar)
c-----!solid solution data
      dimension ixhws(nxtpar)
      dimension ixhit(nxtpar)
c-----!affmul is 1/afcnst; ixplac, etc for sol soln
      save ihws, iplace, ixhws, ixplac, nlu, nerr, ictr, affmul
      save ihit, ixhit
      data ictr/0/, ihit/nmtpar*0/, ixhit/nxtpar*0/

      if(kstep.eq.1) then
        affmul = 1./afcnst
        iplace = 1
        ixplac = 1
c-----!if the file exists, destroy it
        inquire(file='hwsdata', exist=qex)
        if(qex) then
          call getlu(nlu, nerr)
          open(unit=nlu, status='old', file='hwsdata')
          close(unit=nlu, status='delete')
        endif
c-----!find an open device--use EQ3/6 getlu()
        call getlu(nlu, nerr)
c-----!BEGIN_MACHINE_DEPENDENT_CODE_LAHEY
        open(unit=nlu, access='transparent', status='unknown',
          &      file='hwsdata')
c-----!END_MACHINE_DEPENDENT_CODE_LAHEY
c-----!*****Header; logicals implicitly 4bytes*****
c-----!write database name size, then name
        write(nlu) len(utitld(1)), utitld(1)
c-----!write 1st line of input file

```

```

        write(nlu) len(utitl1(1)), utitl1(1)
        write(nlu) qdump, qnochb
c-----!Write number of active...
        write(nlu) kct, jgt, jmt, jst, jxt
c-----!Write the # reactants and the reactant names
        write(nlu) nrct
        do 20 i=1,nrct
            if(jcode(i).eq.1) then
                write(nlu) usolx(nrndex(i))
            else
                write(nlu) ureac(i)
            endif
20        continue
c-----!Element, species, mineral names for log Q/K, gas names
        do 21 i=1,nct
            if(jcflag(i).gt.0) write(nlu) uelem(i)
21        continue

        do 22 i=1,nst
            if(jsflag(i).le.0) write(nlu) uspec(i)
22        continue

        do 23 i=1,nmt
            if(jmflag(i).le.0) write(nlu) umin(i)
23        continue

        do 24 i=1,nxt
            if(jxflag(i).le.0) write(nlu) usolx(i)
24        continue

        do 25 i=1,ngt
            if(jgflag(i).le.0) write(nlu) ugas(i)
25        continue
        endif
c-----END of HEADER BLOCK-----
        if(kstep.eq.-1) then
c-----!append the min names and number of minerals
            if(iplace.gt.1) write(nlu) (umin(ihws(i)), i=1,iplace-1)
c-----!Last 16 bytes are the # min, # sol soln, and # plot points
c-----!and a distinctive tag if last step gets written
            iitag = 123456789
            if(ixplac.gt.1) write(nlu) (usolx(ixhws(i)), i=1,ixplac-1)
            write(nlu) iplace - 1, ixplac - 1, ictr, iitag
            close(nlu)
        else
            write(*,*) 'step=',kstep
c-----!Write data for this step
            ictr = ictr + 1
c-----!calculate the ph, eh
            ph = -actlg(nmhydr)
            if(.not.qnochb) then
                eh = ehfac*0.25*(fo2lg - 4.*ph - 2.*actlg(1) - xxlkeh)
            else
                eh = -999.
            endif
c-----!write out the "master" variables; add tempc, press...
            write(nlu) ph,eh,fo2,xxi,zil,time,tempc,press
c-----!write out amounts of destroyed reactants
            write(nlu) (modr(i), i=1,nrct)
c-----!write out element, species, Q/K, gas data for this step
            do 31 i=1,nct

```

```

        if(jcflag(i).gt.0) write(nlu) mteaq(i)
31      continue

        do 32 i=1,nst
          if(jsflag(i).le.0) write(nlu) conc(i)
32      continue

        do 33 i=1,nmt
          if(jmflag(i).le.0) write(nlu) aff(i)*affmul
33      continue

        do 35 i=1,ngt
          if(jgflag(i).le.0) write(nlu) fug(i)
35      continue

c-----!update ihws array and write current step data
        do 100 i=1,nmt
          if((jmflag(i).eq.-1).and.(ihit(i).eq.0)) then
            ihit(i) = 1
            ihws(iplace) = i
            iplace = iplace + 1
          endif
100      continue
c-----!write this step's mineral amount data
        write(nlu) iplace-1
        if(iplace.gt.1) write(nlu) (momn(ihws(i)), i=1,iplace-1)

c-----!update ixhws array and write current step data
        do 200 i=1,nxt
          if((jxflag(i).eq.-1).and.(ixhit(i).eq.0)) then
            ixhit(i) = i
            ixhws(ixplac) = i
            ixplac = ixplac + 1
          endif
200      continue
c-----!write this step's sol soln amount data
        write(nlu) ixplac-1
        if(ixplac.gt.1) write(nlu) (motx(ixhws(i)), i=1,ixplac-1)
      endif
    end

```

Place the following statement in the EQ6 **path()** routine, immediately after the statement at label 20 (20 kstep=kstep+1):

```
      call hws4io(kstep, xi, xlkeh, nhydr)
```

then place the following 2 statements in **path()**, between the "999 continue" and "end" statements:

```
      call hws4io(kstep, xi, xlkeh, nhydr)
      call hws4io(-1, xi, xlkeh, nhydr)
```

and recompile EQ6 according to the instructions in the EQ3/6 release notes.

Distribution

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