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CHEMFORM
User's Guide

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MANAGED BY
MARTIN MARIETTA ENERGY SYSTEMS, INC.
FOR THE UNITED STATES
DEPARTMENT OF ENERGY

ORNL/GWPO-0010

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USER'S GUIDE

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January 1996

Prepared by
Environmental Sciences Division
Oak Ridge National Laboratory

Prepared for the
U.S. Department of Energy

Under budget and reporting code 26 45 02 00 0
Office of Environmental Restoration and Waste Management
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37831-6285
managed by
LOCKHEED MARTIN ENERGY RESEARCH, CORP.
For the
U.S. DEPARTMENT OF ENERGY
under contract DE-AC05-96OR22464

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1. INTRODUCTION

CHEMFORM is a DOS-based program which converts geochemical data files into the format read by the U.S. Geological Survey family of models: WATEQ4F (Ball et al., 1991), PHREEQE (Parkhurst et al., 1980), or NETPATH (Plummer et al., 1991). These geochemical models require data formatted in a particular order, which typically does not match data storage. CHEMFORM converts geochemical data that are stored in an ASCII file to input files that can be read by these models, without being re-entered by hand. The data may be in any order and format in the original file, as long as they are separated by blanks. The location of each data element in the input file is entered in CHEMFORM. Any required data that are not present in your file may also be entered. The positions of the data in the input file are saved to be used as defaults for the next run.

CHEMFORM runs in two modes. In the first mode, it will read one input file and write one output file. The input file may contain data on multiple lines, and the user will specify both line number and position of each item in CHEMFORM. This mode facilitates the conversion of the input from one model to the format needed by another model. In the second mode, the CHEMFORM input files contains more than one water analysis. All the geochemical data for a given sample are stored on one line, and CHEMFORM writes an output file for each line. This mode is useful when many samples are available for a site in the same format (different monitoring points or samples taken at different times from one monitoring point). Re-entering large data sets can lead to errors. It may be necessary to create two input files to contain all the geochemical data for a sample. For example, if the original format is a database or spreadsheet, they may be limited in the number of characters per record which they will write to an ASCII. For example, Lotus-123™ will only write ASCII records up to 240 characters long. When more that 240 characters worth of data need to be processed, they can be processed as two files. One of the input files contains the chemical concentrations and the second file contains any other required data (such as concentration units). Each line of the two CHEMFORM input files is matched in the same line order to create a single water sample record. CHEMFORM processes each line and writes as many files as there are lines.

CHEMFORM is distributed on a single high-density diskette or through anonymous ftp (ftp.esd.ornl.gov or brrcrftp.cr.usgs.gov). It should be installed by creating a new directory on your hard disk and copying the files on the distribution diskette to that directory. It requires about 480K of free memory. Loading the program and data requires about 400K of hard disk space. Both the keyboard and mouse may be use in data input.

This document is a user's guide for CHEMFORM and provides a brief documentation of that program. It is assumed that the user already knows how to run WATEQ4F, PHREEQE, and

NETPATH, understands the meanings of the data entered for them, and is familiar with geochemistry and geochemical modeling.

2. USER'S GUIDE

Start CHEMFORM by typing "chemform". The files CHEMFORM.EXE, CHEMFORM.VVD, CHEMFORM.CHO, and CONCPOS.DAT must be present in the directory, along with initial default files for input screens.

If you are using a monochrome monitor with a color display card, type 'mode bw80' before starting the program to make the screens easier to read. Navigation in CHEMFORM is simple. Menu selections are made either with the mouse, by pressing the key letter of the choice, or by using the arrow keys to position on the choice and pressing the <Enter> key. Move through the data entry screens with a mouse, the arrow keys, or the <Enter> or <Tab> key. Exit a data entry screen by clicking the Exit push button with a mouse or by pressing the <F10> key. The special functions of keys on data entry screens are listed in Table 1.

Table 1. Special Key Functions

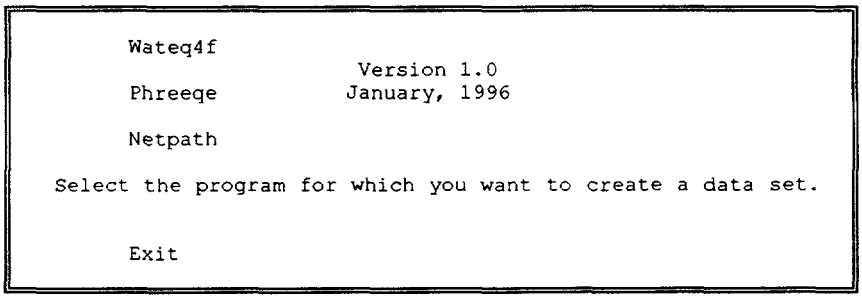
Key	Action
up	Moves to the next item located physically above the current one
down	Moves to the next item located physically below the current one
Enter	Moves to the next item on the screen
Esc	Returns you to the first (model selection) screen
F2	Re-displays the choice list, if available.
Shift-F3	Redisplays the original value in the field
F6	Clears the field
Shift-F6	Clears from the cursor to the end of the field
F7	Moves to the previous screen
F8	Moves to the next item on the screen
F10	Exits the current screen
Tab	Moves to the next item on the screen
Shift-Tab	Moves to the previous item on the screen
Ctrl-End	Moves to the last item on the screen
Ctrl-Home	Moves to the first item on the screen

Note that CHEMFORM does no error checking. It is assumed that the data positions that you enter are available selections. If you enter the same position for two data items or if you enter position data that causes CHEMFORM try to read a number from a non-numeric field, or causes CHEMFORM to try to read, for example, the sixth item on a line with only two items present, several things may happen. (1) You may need to re-boot your computer. (2) Your data files will

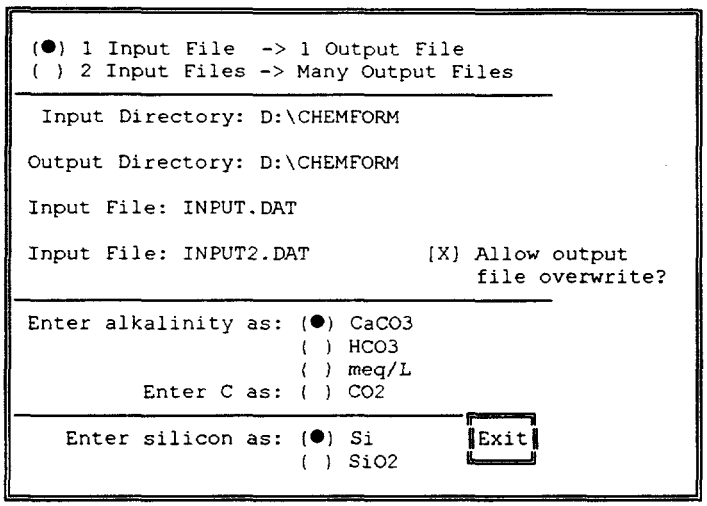
contain garbage. (3) Your default files will contain garbage. This behavior is not due to bugs in CHEMFORM; it is an indication that you need to re-enter data positions that are in error.

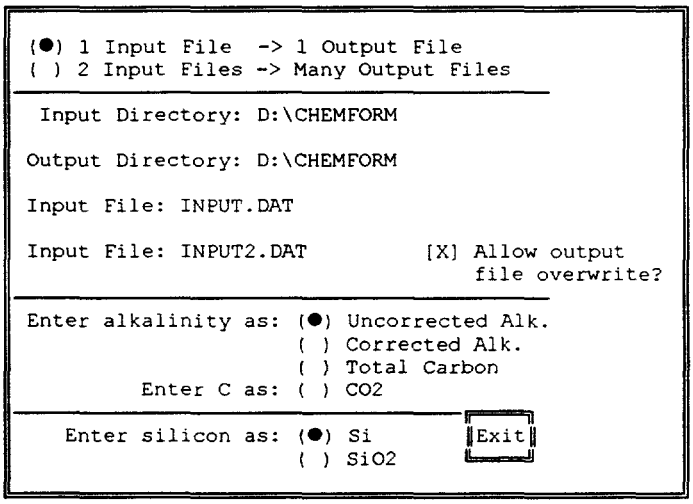
2.1 Initial Screens

The first screen that you see, shown below, allows you to select the model for which you want to create an input file.



You are returned to this screen after you are finished entering data and your new files are created. You exit CHEMFORM from this screen. When you select a model, one of the following screens pops up, depending on alkalinity options in the different models.





The screen on the left is for WATEQ4F and PHREEQE. The screen on the right is for NETPATH. On these screens you select several options and enter the location of your input and output files.

First select the input mode that you want to use. Click the mouse on your choice or use the arrow keys to mark your selection and press <Enter> to continue.

Second, enter the names of the directories and select from available input files. If you select the first mode, only the first input file is used; if you select the second mode, both input files are used. Although you can use the same name for both files, if two files are needed because of long record length, the first file should contain data described in section 2.2 and the second file data in section 2.3.

Third, for the '2 Input Files ->Many Output Files' only, you may select to allow or disallow the overwriting of output files. For the '1 Input File -> Output File' choice, file overwriting is always allowed.

Fourth, select how alkalinity will be entered. These alkalinity options are reviewed in the manuals of the geochemical models. Click the mouse on your choice or use the arrow keys to mark your selection and press <Enter> to continue. Note that if you select meq/L, the rest of your concentration data should be in these units as well. Also, the 'Enter C as CO2' choice is not available for NETPATH.

Fifth, select how silicon will be entered. Click the mouse on your choice or use the arrow keys to mark your selection and press <Enter> to continue.

Exit this screen by pressing the <F10> key or clicking the mouse on the Exit push button. When you exit this screen, you will see either the NETPATH, PHREEQE, or WATEQ4F input screens, depending on which one you selected.

2.2 Input of Data Other than Concentrations

Two data entry screens are used to enter the data other than concentrations. The appearance of these screens is different for each geochemical model, but the use of them is the same.

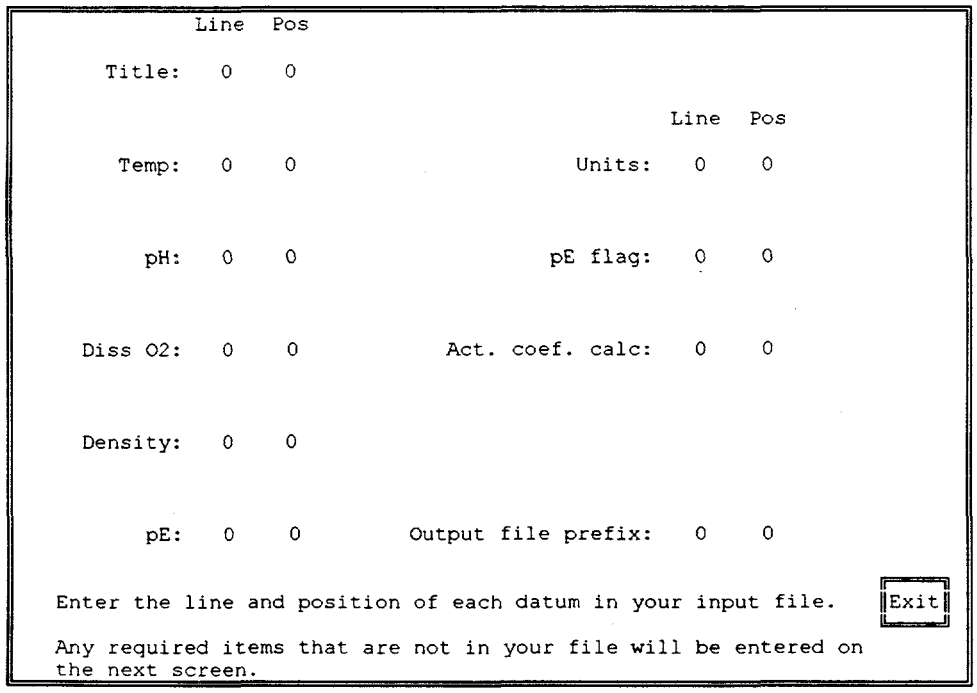
On the first screen you enter the position of each of the data items. If you have selected the '1 Input File ->1 Output File' mode, you will enter the line each item appears on in your file and the position of that item within the line. The first item in the file is at line 1, position 1 (not 0, 0). The position is the item count on that line, where each item is delimited by blanks. For example the 'pos' value for the word 'position' in the first line of this paragraph is 8. If you have selected in '2 Input Files -> Many Output Files' mode, then you only enter the position of each item within each line. Leave zeros for any items that will not be read from your input file. Note that the title is read as a full line in '1 Input File ->1 Output File' mode, but as one word in '2 Input Files -> Many Output Files' mode. This means that the title is the only data item that can be read from the title line in '1 Input File ->1 Output File' mode.

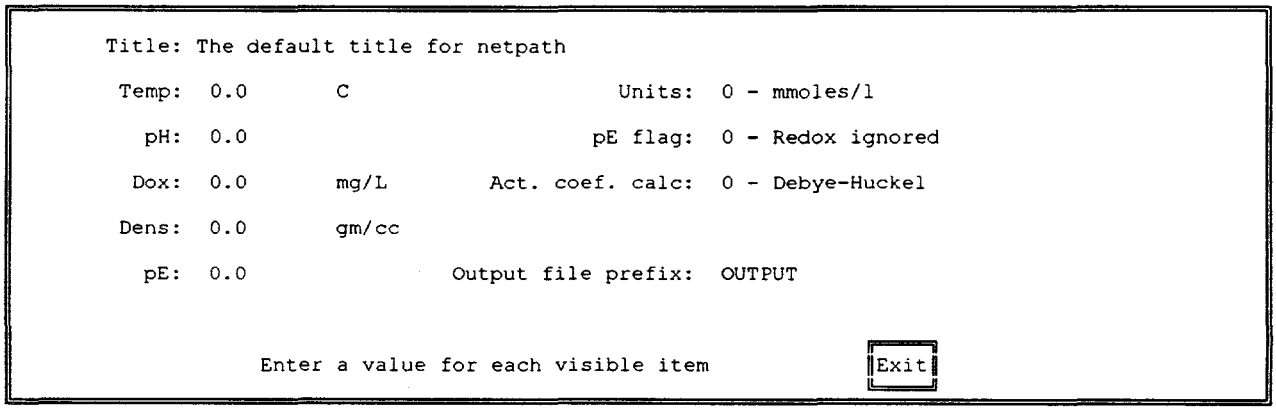
The second screen that appears allows you to enter values for any data that was not given a line and position on the first screen; that is any item with a 0 for line or position. Real numbers may be entered with an exponent. Range checks are performed on data that allow integer only values.

Note that the output file prefix may be read from the data (for example, the well name) or may be entered by hand. The suffix of the output file is .PAT, .PHR, or .WAT, depending on the geochemical model selected. In '1 Input File -> 1 Output File' mode no check is made whether or not the output file exists, and so may overwrite an existing file. In '2 Input Files -> Many Output Files' mode, existence of the output file is checked when the option to allow overwriting is not selected, and if that name already exists, a number from 2 to 99 is appended to the file name to make it unique. This feature provides new names for monitoring points sampled at different times. An option in the first screen allows the users to overwrite existing file names.

Note, however, that if you select the '2 Input Files -> Many Output Files' mode, it is possible to overwrite your output file with a file of the same name even through the overwrite option has not been selected. Since DOS only allows eight character file name prefixes, if your selected file name has eight characters, the number that the program appends will be truncated from the name, and your output file will be over- written.

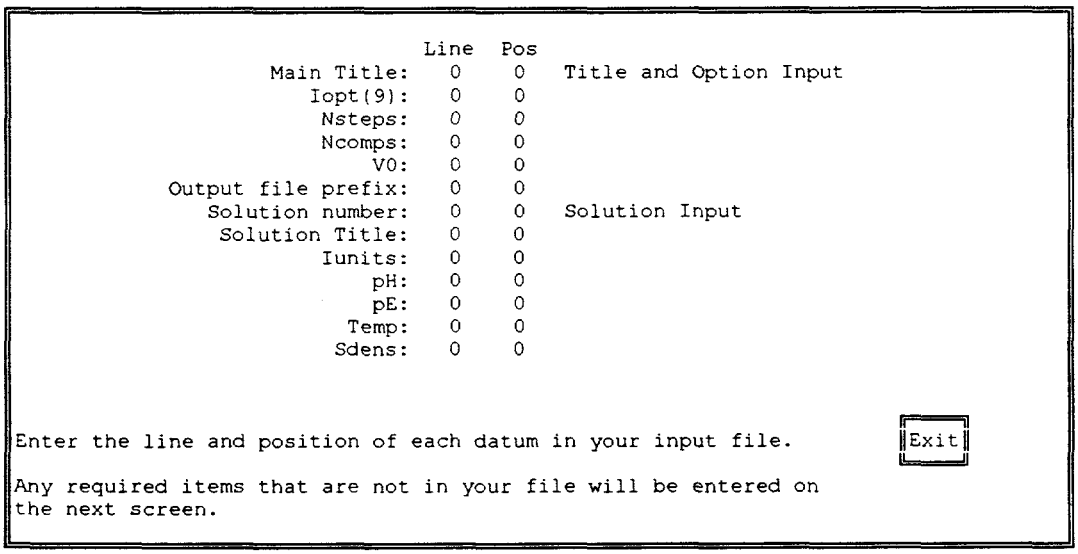
The two NETPATH input screens are shown below.

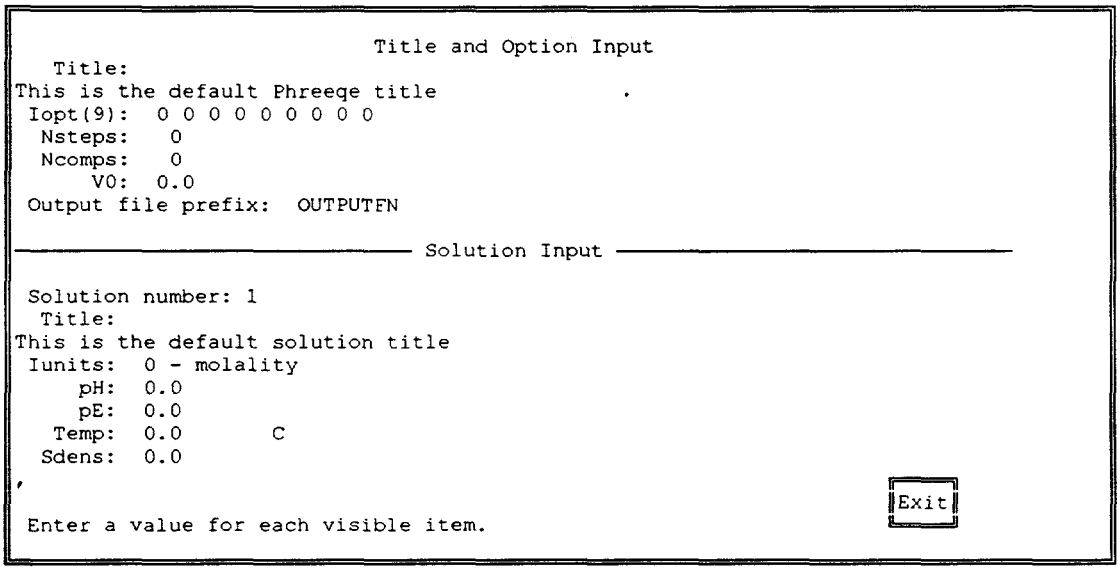




Note that the three top items on the right are entered from choice lists.

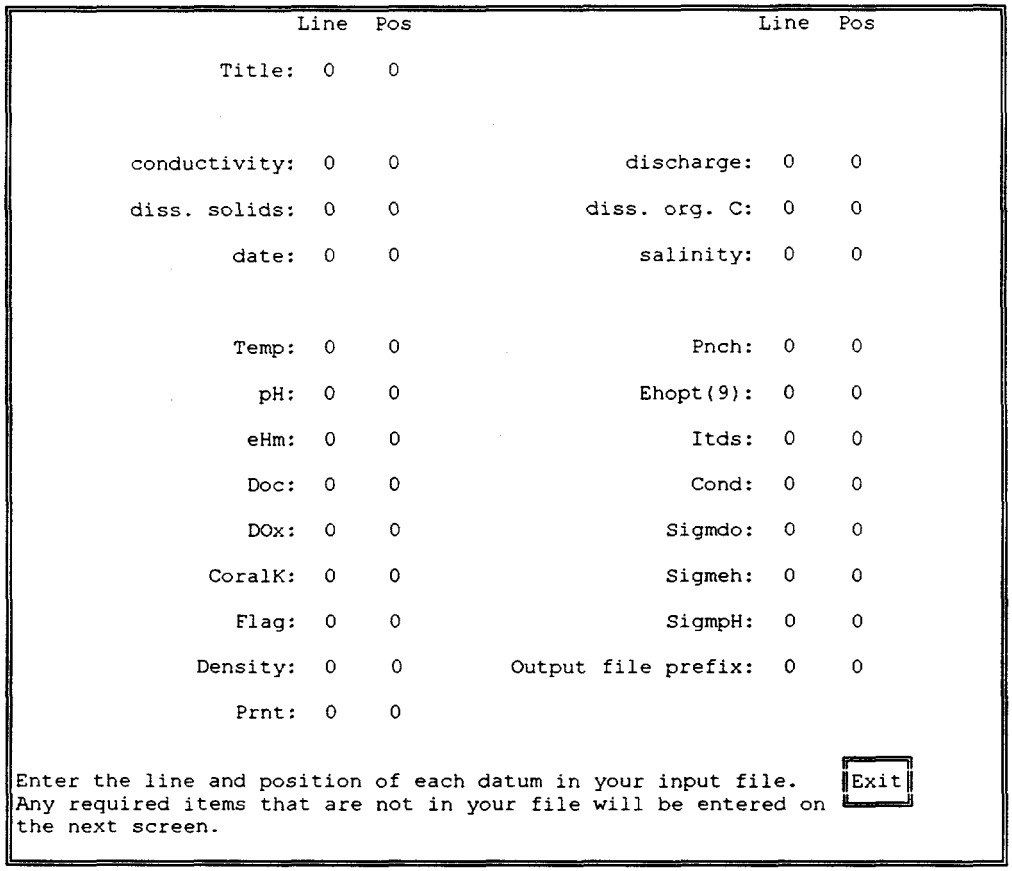
The two PHREEQE input screens are shown below.





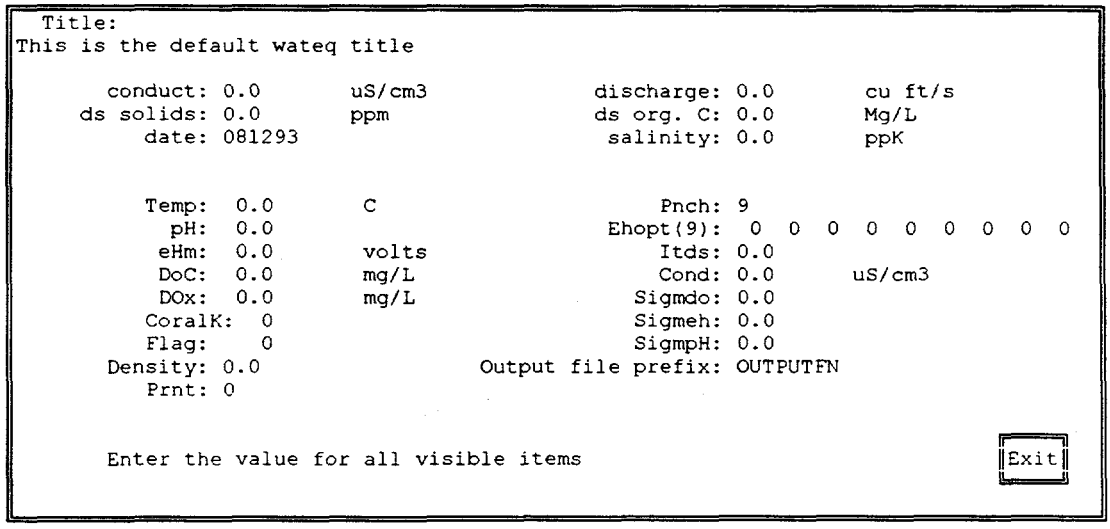
Note that PHREEQE variables IALK and NTOTS are computed internally, based on other data entered.

The two WATEQ4F input screens are shown below.



	Line	Pos		Line	Pos
Title:	0	0			
conductivity:	0	0	discharge:	0	0
diss. solids:	0	0	diss. org. C:	0	0
date:	0	0	salinity:	0	0
Temp:	0	0	Pnch:	0	0
pH:	0	0	Ehopt(9):	0	0
eHm:	0	0	Itds:	0	0
Doc:	0	0	Cond:	0	0
DOx:	0	0	Sigmdo:	0	0
CoralK:	0	0	Sigmeh:	0	0
Flag:	0	0	SigmpH:	0	0
Density:	0	0	Output file prefix:	0	0
Prnt:	0	0			

Enter the line and position of each datum in your input file. Any required items that are not in your file will be entered on the next screen. [Exit]



Title:
This is the default wateq title

conduct:	0.0	uS/cm3	discharge:	0.0	cu ft/s
ds solids:	0.0	ppm	ds org. C:	0.0	Mg/L
date:	081293		salinity:	0.0	ppK
Temp:	0.0	C	Pnch:	9	
pH:	0.0		Ehopt(9):	0 0 0 0 0 0 0 0 0	
eHm:	0.0	volts	Itds:	0.0	
DoC:	0.0	mg/L	Cond:	0.0	uS/cm3
DOx:	0.0	mg/L	Sigmdo:	0.0	
CoralK:	0		Sigmeh:	0.0	
Flag:	0		SigmpH:	0.0	
Density:	0.0		Output file prefix:	OUTPUTFN	
Prnt:	0				

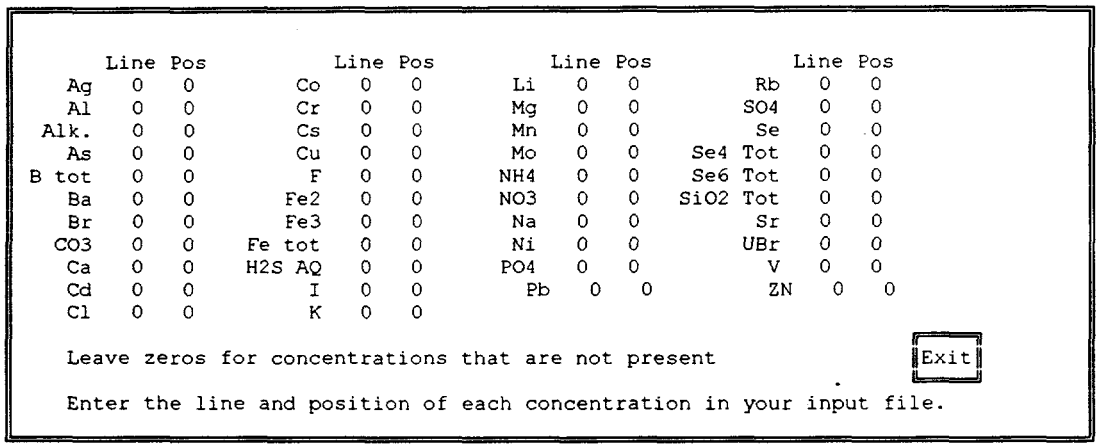
Enter the value for all visible items [Exit]

Note that if the date field in your data contains more than 6 characters, the format of the files that you write will be incorrect.

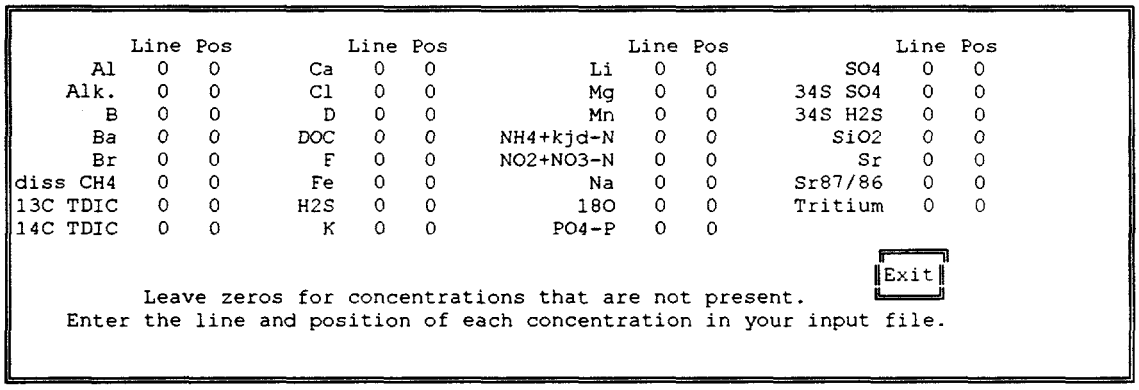
Following this pair of screens, you will see the chemical concentration screen.

2.3 Concentration Input

The following screens are used to enter the chemical concentration positions. The first appears after the WATEQ4F or PHREEQE screens shown in the previous section. The second appears after the NETPATH screens.



	Line	Pos		Line	Pos		Line	Pos		Line	Pos
Ag	0	0	Co	0	0	Li	0	0	Rb	0	0
Al	0	0	Cr	0	0	Mg	0	0	SO4	0	0
Alk.	0	0	Cs	0	0	Mn	0	0	Se	0	0
As	0	0	Cu	0	0	Mo	0	0	Se4 Tot	0	0
B tot	0	0	F	0	0	NH4	0	0	Se6 Tot	0	0
Ba	0	0	Fe2	0	0	NO3	0	0	SiO2 Tot	0	0
Br	0	0	Fe3	0	0	Na	0	0	Sr	0	0
CO3	0	0	Fe tot	0	0	Ni	0	0	UBr	0	0
Ca	0	0	H2S AQ	0	0	PO4	0	0	V	0	0
Cd	0	0	I	0	0	Pb	0	0	ZN	0	0
Cl	0	0	K	0	0						



	Line	Pos		Line	Pos		Line	Pos		Line	Pos
Al	0	0	Ca	0	0	Li	0	0	SO4	0	0
Alk.	0	0	Cl	0	0	Mg	0	0	34S SO4	0	0
B	0	0	D	0	0	Mn	0	0	34S H2S	0	0
Ba	0	0	DOC	0	0	NH4+kjd-N	0	0	SiO2	0	0
Br	0	0	F	0	0	NO2+NO3-N	0	0	Sr	0	0
diss CH4	0	0	Fe	0	0	Na	0	0	Sr87/86	0	0
13C TDIC	0	0	H2S	0	0	18O	0	0	Tritium	0	0
14C TDIC	0	0	K	0	0	PO4-P	0	0			

On these screens you enter the location of each concentration. There are fewer chemicals available for PHREEQE than for WATEQ4F. You cannot enter concentration values in CHEMFORM. You can, of course, edit the files written by CHEMFORM to include any concentrations, or other data, not present in you input file.

When you exit these screens, your new data files are created, and then you will be returned to the initial menu, where you can process another file or exit CHEMFORM.

3. DATA FILES

There are few constraints on the files that you use as input. Keep in mind that CHEMFORM reads all data, except for the title, as delimited by blanks, so that a name entered as A. B. Smith is treated as three data items; A.B.Smith as one. A title is read as a single line in '1 Input File -> 1 Output File' mode, but is read as a single data item in 2 files -> many files mode. Also remember that in '2 Input Files -> Many Output Files' mode, there must be exactly the same number of data items on each line of each file and all the data values used must be valid input. Missing values in a database should not be extracted as blanks.

Output files are ready to be used as input to the appropriate model. NETPATH requires one extra step. In your NETPATH directory there is a file called NETPATH.FIL. You must add your data file prefix to this file or use the NETPATH.FIL file that is written by CHEMFORM, which contains the prefixes of the files that it has written. Note that running CHEMFORM bypasses the DB program in NETPATH. CHEMFORM performs the DB function of NETPATH: it executes the portion of NETPATH that creates WATEQ input and creates the NETPATH files *.in, *.out and *.pat.

Because NETPATH requires more than one set of data in an input file, CHEMFORM actually writes the output of the '2 Input Files -> Many Output Files' mode to one file for NETPATH. If you use the '1 Input File -> 1 Output File' mode for NETPATH, you will have to concatenate the resulting single output file with other NETPATH data.

Eight data files are provided with CHEMFORM. They are listed in Table 2. The default files contain any data and data location that where entered during the previous CHEMFORM run. If your data files are in a few standard formats, it may be worthwhile to save multiple copies of the default files, and copy the one you want to the '.DEF' file as needed. The '.SAV' files contain all zeros and are provided so that when you enter your position data so incorrectly that the default file cannot be read, you have a place to start over.

Table 2. CHEMFORM Data Files

File	Purpose
CONCPOS.DAT	Stores indices of chemicals used by the geochemical models
NETPATH.DEF	Stores defaults for NETPATH input screens
PHREEQE.DEF	Stores defaults for PHREEQE input screens
WATEQ.DEF	Stores defaults for WATEQ4F input screens
NETPATH.SAV	Stores initial defaults for NETPATH input screens; all data set to zero
PHREEQE.SAV	Stores initial defaults for PHREEQE input screens; all data set to zero
WATEQ.SAV	Stores initial defaults for WATEQ4F input screens; all data set to zero
WATEQF.DAT	Required for NETPATH only to run WATEQ

4. PROGRAM FILES

CHEMFORM consists of six files of C code, which provide the user interface, and two files containing Fortran subroutines from the NETPATH DB program, which run WATEQ4F and write the NETPATH input file. The user interface also uses the Vermont Views™ library routines to produce the screens shown. Minor changes were made to the NETPATH DB Fortran files to interface them to the C code. CHEMFORM was compiled using the Microsoft Fortran version 5.1 and C version 6.0 compilers.

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