



NetpathXL—An Excel[®] Interface to the Program NETPATH

By David L. Parkhurst and Scott R. Charlton

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By David L. Parkhurst and Scott R. Charlton

Abstract

NetpathXL is a revised version of NETPATH that runs under Windows[®] operating systems. NETPATH (Plummer and others, 1991, 1994) is a computer program that uses inverse geochemical modeling techniques to calculate net geochemical reactions that can account for changes in water composition between initial and final evolutionary waters in hydrologic systems. The inverse models also can account for the isotopic composition of waters and can be used to estimate radiocarbon ages of dissolved carbon in ground water. NETPATH relies on an auxiliary, database program, DB, to enter the chemical analyses and to perform speciation calculations that define total concentrations of elements, charge balance, and redox state of aqueous solutions that are then used in inverse modeling. Instead of DB, NetpathXL relies on Microsoft Excel[®] to enter the chemical analyses. The speciation calculation formerly included in DB is implemented within the program NetpathXL. A program DBXL can be used to translate files from the old DB format (*.lon* files) to NetpathXL spreadsheets, or to create new NetpathXL spreadsheets. Once users have a NetpathXL spreadsheet with the proper format, new spreadsheets can be generated by copying or saving NetpathXL spreadsheets. In addition, DBXL can convert NetpathXL spreadsheets to PHREEQC (Parkhurst and Appelo, 1999) input files. New capabilities in PHREEQC (version 2.15) allow solution compositions to be written to a *.lon* file, and

inverse models developed in PHREEQC to be written as NetpathXL *.pat* and model files. NetpathXL can open NetpathXL spreadsheets, NETPATH-format path files (*.pat* files), and NetpathXL-format path files (*.pat* files). Once the speciation calculations have been performed on a spreadsheet file or a *.pat* file has been opened, NetpathXL performs almost identically to the original NETPATH. Development of models and viewing results in NetpathXL rely on keyboard entry as in NETPATH.

Introduction

NETPATH (Plummer and others, 1991, 1994) is an interactive Fortran 77 computer program used to interpret net geochemical mass-balance reactions between initial (or multiple initial waters that mix) and final waters along real or hypothetical flow paths in aquifers or other hydrologic systems. The program uses inverse geochemical modeling techniques (Plummer and others, 1983; Plummer 1985; Parkhurst and Plummer, 1993; Glynn and Brown, 1996; Nordstrom, 2007) to construct geochemical reaction models by using chemical and isotopic data for waters from the hydrochemical system. The inverse model is a set of mixing fractions and mole transfers that exactly account for the changes in concentration of elements in the waters. Inverse models between selected evolutionary waters are found for every possible combination of the plausible phases that can account for the composition of a selected set of chemical and isotopic constraints in the system. The processes of dissolution, precipitation, ion exchange, oxidation/reduction, degradation of organic compounds, incongruent reaction, gas exchange, mixing, evaporation, and dilution are included. It also is possible to account for changes in isotopic compositions of six elements: hydrogen (deuterium and tritium) and oxygen isotopic evolution is accounted for by mixing of waters (no fractionation or mineral mass transfer); carbon (carbon-13 and carbon-14), sulfur, nitrogen, and strontium isotopic evolution is accounted for by mixing, mineral mass transfer, isotopic fractionation, and isotopic exchange. Finally, the inverse models can be used to adjust radiocarbon data for geochemical reaction effects and refine estimates of radiocarbon age. The

NETPATH software includes a data-base program, DB, for storing and editing chemical and isotopic data for use in NETPATH.

NETPATH has been used to investigate geochemical and isotopic reactions in a large number of hydrologic systems for more than 15 years (see for example: Plummer and others, 1990; Aravena and others, 1995; Plummer and Sprinkle, 2001). The modeling concepts in NETPATH can be traced to geochemical mass-balance calculations originally demonstrated by Garrels and Mackenzie (1967), and have evolved through a series of theoretical (Plummer and Back, 1980; Plummer and others, 1983; Plummer, 1992; Glynn and Plummer, 2005; Parkhurst, 1997) and software contributions (Plummer and others, 1975; Parkhurst and others, 1982; Plummer and others, 1991, 1992, 1994).

More recently, inverse geochemical modeling has been incorporated into the geochemical model PHREEQC (Parkhurst and Appelo, 1999) and its graphical user interface PhreeqcI (Charlton and Parkhurst, 2002) and into a spreadsheet program, SpreadBal (Bowser and Jones, 2002a, 2002b). Advantages and limitations of the NETPATH and PhreeqcI inverse modeling capabilities are discussed in Glynn and Brown (1996) and Glynn and Plummer (2005). NETPATH, PHREEQC (and PhreeqcI), and SpreadBal are all capable of performing basic inverse modeling. The strengths of each program are as follows: NETPATH allows for isotope fractionation, radiocarbon dating, isotope mole balance, and redox processes. SpreadBal primarily is designed for aluminosilicate and clay reactions, with special emphasis on the variable compositions of these minerals. PHREEQC considers uncertainties in analytical data for elements and isotopes; it considers redox processes and isotope mole balance, but not isotope fractionation or radiocarbon dating.

The data entry program for NETPATH, DB, requires editing data one piece at a time. DB saves data in two formats: the *.lon* file contains the raw concentration data and the *.pat* file contains selected results from speciation calculations performed by DB (total concentrations of elements, redox state, and isotopic compositions). NETPATH reads the *.pat* file to obtain the data needed for inverse modeling.

Since the original publication of NETPATH, advances in computer technology permit replacement of the DB data-entry style with the universally familiar spreadsheet. NetpathXL is a revised version of NETPATH that can read an Excel spreadsheet that contains the raw concentration data. The speciation calculation, formerly in the program DB, has been moved to the program NetpathXL. Each time NetpathXL reads a NetpathXL spreadsheet, speciation calculations are performed and a *.pat* file is written; although the format of a *.pat* file written by NetpathXL differs from one written by DB, NetpathXL can read data from a *.pat* file created by either DB or NetpathXL.

The NetpathXL spreadsheet has a fixed set of columns and header rows (see appendix 2). The program DBXL generates a spreadsheet of the proper format, into which raw concentration and isotopic data can be entered. DBXL also can translate a *.lon* file [written by NETPATH or PHREEQC (version 2.15 or later)] to a NetpathXL spreadsheet. Additional NetpathXL spreadsheets can be generated by copying old spreadsheets and clearing the concentration data. New chemical and isotopic data can be entered cell-by-cell or copied and pasted from other spreadsheets or files into NetpathXL spreadsheets.

New capabilities have been added to facilitate the interchange of data between PHREEQC and DBXL and NetpathXL. DBXL can read the data from a NetpathXL spreadsheet and write a file with all of the solution definitions that is readable by PHREEQC (*.pqi* file). Thus, PHREEQC can be used to calculate inverse models or forward models by using data that was entered for NetpathXL. In addition, PHREEQC (version 2.15 and later) can write files that are readable by DBXL and NetpathXL. The solution data defined in PHREEQC (**SOLUTION**, **SOLUTION_SPREAD**, and **SAVE solution**) can be written to a *.lon* file by using the `-lon_netpath` identifier in the **INVERSE_MODELING** data block. This file can be read by DBXL and converted into a NetpathXL spreadsheet. In addition, PHREEQC inverse models can be saved as *.pat* and model files by using the `-pat_netpath` identifier in the **INVERSE_MODELING** data block. PHREEQC adjusts concentrations in the process of finding inverse models. The *.pat* file written by PHREEQC contains these adjusted concentrations for each

solution for each model, and each model is written to a NetpathXL model file that can be read by NetpathXL. By using these files, NetpathXL can reproduce exactly a PHREEQC inverse model. This capability is useful, for example, if inverse model development is done in PHREEQC, but radiocarbon age dating is done with NetpathXL.

Installing NetpathXL and DBXL

NetpathXL and DBXL use Microsoft Excel to store and retrieve data. Excel must be accessible on the computer on which NetpathXL and DBXL are installed.

Download the latest version from http://www.brr.cr.usgs.gov/projects/GWC_coupled/netpath. The file will have the extension *.msi*, and can be installed by using the Windows Installer, which is available automatically in Windows XP and higher. As administrator, simply double click on the downloaded *.msi* file. The programs will be installed in the *C:\Program Files* directory by default. It is possible to install as a non-administrator if a different directory is selected. Once installed, the programs can be run through the Start Menu at the bottom left corner of the screen.

The programs normally are installed in the directory *c:\Program Files\USGS\NetpathXL*. Within this directory are subdirectories: *bin*, which contains the executables for NetpathXL and DBXL; *database*, which contains the database for the speciation model, *db.dat*, and the database of mineral stoichiometries, *netpath.dat*; *doc*, which contains PDF versions of this report and the documentation for NETPATH (Plummer and others, 1994); and *examples*, which contains the data and model files for the examples described in the NETPATH documentation (Plummer and other, 1994).

Using DBXL

DBXL can be executed from the Windows start menu at the bottom left of the screen or by browsing for the executable file (*c:\Program Files\USGS\NetpathXL\bin\dbxl.exe*) and double clicking.

The user may want to add a desktop icon by right clicking on the start-menu item or the executable file (Send To->Desktop). When the program starts, a screen (fig. 1) appears that has five options: (1) create a spreadsheet from the data in a *.lon* file that has been written by DB, (2) open a NetpathXL spreadsheet (*.xls* suffix), (3) create an empty NetpathXL spreadsheet, (5) create a PHREEQC input file (*.pqi*) from a NetpathXL spreadsheet file, or (5) exit DBXL. Options are selected by typing 1, 2, 3, 4, or 5 followed by enter. Selecting options 1, 2, 3, or 4 will start the standard Windows file browser to select the file to be read or to specify the name of the new NetpathXL spreadsheet (fig. 2). For options 1, 2, and 3, after a file has been selected, an Excel session will be started, and DBXL will close. For option 4, after a file has been selected, a PHREEQC *.pqi* file will be written, after which, DBXL will close. Other functionality of DB, including “Check” charge balance and “Print” data reports was not retained in DBXL.

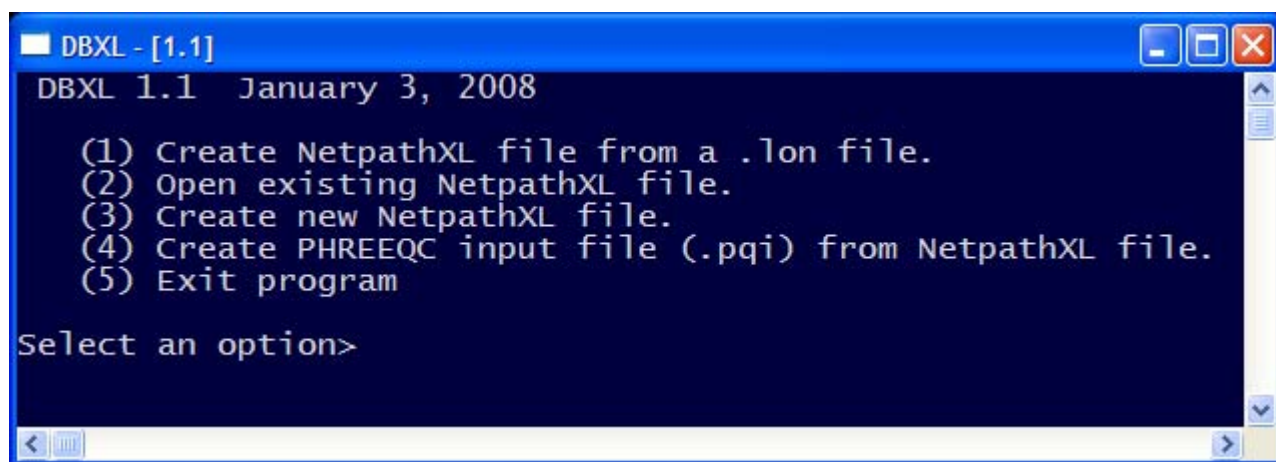


Figure 1. Options screen for DBXL.

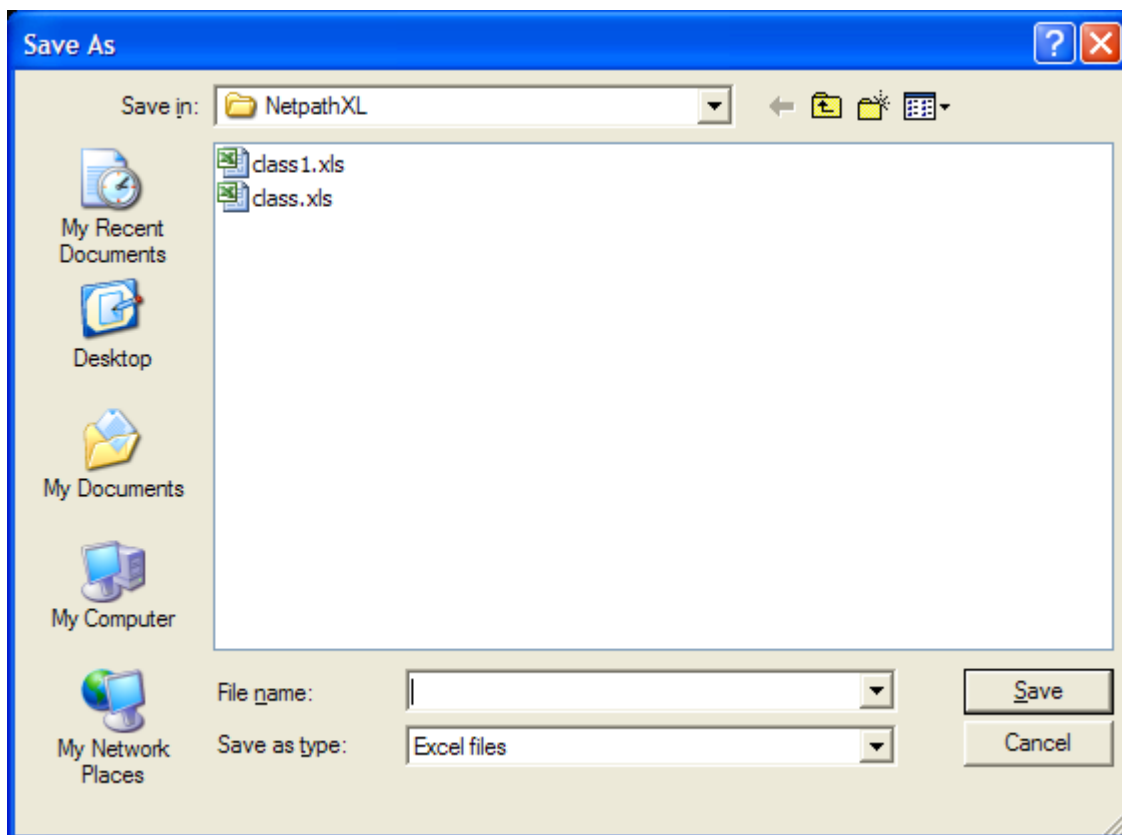


Figure 2. File browser using DBXL option 3.

Using NetpathXL

NetpathXL can be executed from the Windows start menu at the bottom left of the screen or by browsing for the executable file (*c:\Program Files\USGS\NetpathXL\bin\netpathxl.exe*) and double clicking. The user may want to add a desktop icon by right clicking on the start-menu item or the executable file (Send To->Desktop). When the program starts, a screen (fig. 3) appears that has three options: (1) open an existing NetpathXL spreadsheet (*.xls* suffix), (2) open a *.pat* file created by DB or NetpathXL, or (3) exit NetpathXL. Options are selected by typing 1, 2, or 3 followed by enter. Once option 1 or 2 is selected, the standard Windows file browser is used to select a file. After a file has been selected, execution will be essentially the same as the program NETPATH; all options and data entry

are by keystrokes, and the mouse is not functional except to give focus to the NetpathXL window. The working directory will be the directory that contains the file selected by the file browser.

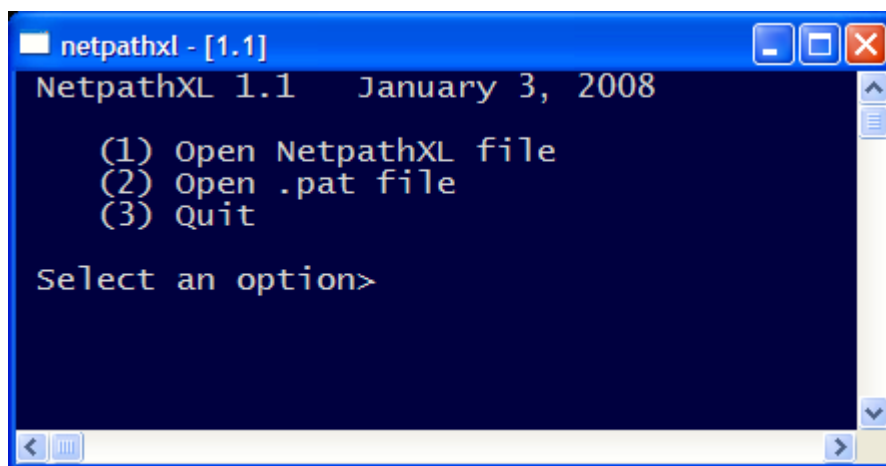


Figure 3. Options screen for NetpathXL.

If a NetpathXL spreadsheet is selected (option 1), a speciation calculation will be performed. A database file named *db.dat* is required for this speciation calculation. The default database file is found in the *database* subdirectory of the installation directory (*c:\Program Files\USGS\NetpathXL\database\db.dat*).

Another file, *netpath.dat*, contains the stoichiometry and isotopic composition of minerals, which are needed for inverse modeling calculations. NetpathXL will look for this file in the working directory (the directory containing the file read at startup). If it is not found in the working directory, the file will be copied from the database subdirectory of the installation directory (*c:\Program Files\USGS\NetpathXL\database\netpath.dat*).

If a NetpathXL spreadsheet is read, one additional option is added to the edit screen that was not in the original NETPATH program. The first option of the edit screen is now “1) Reread Excel file” (fig. 4), which is not available in NETPATH. (The edit screen is invoked by typing “E” or “e” on the main screen of NetpathXL, fig. 5.) This option will reread the last NetpathXL spreadsheet and perform

speciation calculations by using the same options (charge balance option and database file) that were used when the NetpathXL spreadsheet was originally read. (To reread the Excel file, but use different options, select the option “Well file,” which will query for each option.) The current inverse model—wells, phases, constraints, and other options—is retained when the NetpathXL spreadsheet is reread. By using the reread option, concentration or isotopic data can be revised in the NetpathXL spreadsheet and then quickly imported into NetpathXL. Typically, the Excel spreadsheet will be left open and the reread option will be used whenever changes are made to the spreadsheet. Note that the changes to the spreadsheet must be saved (File->Save within Excel) before the spreadsheet is reread. The capability to view Excel while running NetpathXL replaces the <V>iew option of the main screen of NETPATH.

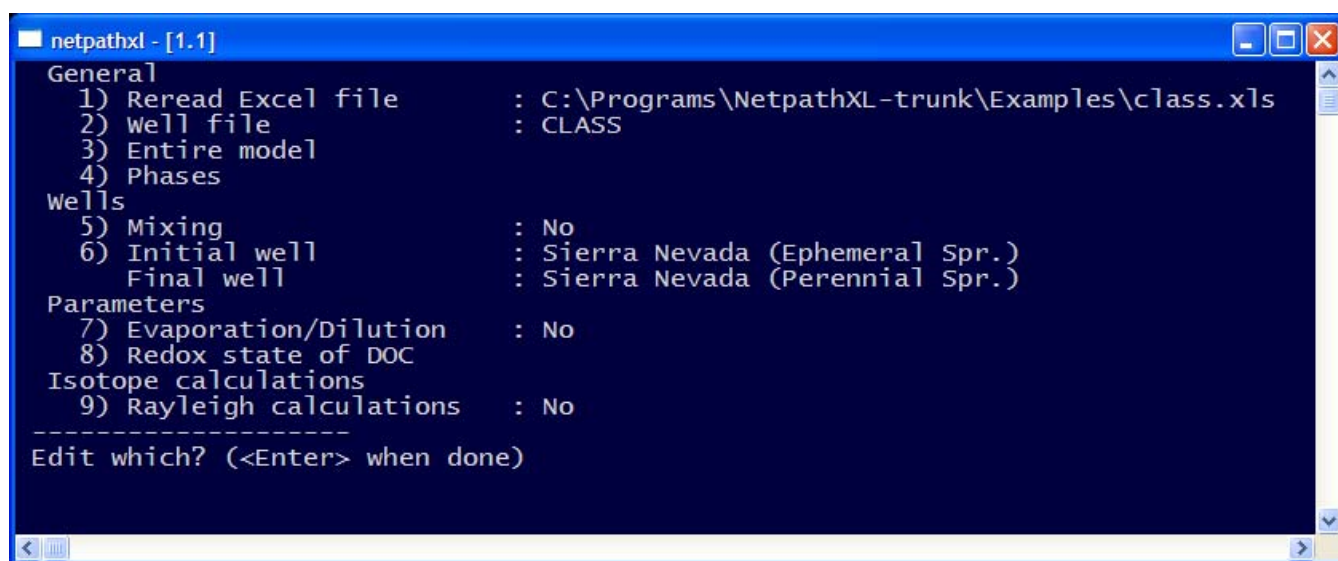


Figure 4. Edit screen for NetpathXL.

One additional option (<F>ont) has been added to the main screen (fig. 5). Typing “F” at the main-screen prompt will result in queries for font height, font brightness, and background brightness. The default font size is 16; specifying a larger or smaller number (8 to 24) correspondingly will increase or decrease the font size used for painting the screens in NetpathXL. The default font brightness is 0.85, increasing or decreasing the number (0.3 to 1.0) correspondingly will bright or dim the font. The default

background brightness is 0.25 (midnight blue); a value of 0 will produce a black background and a value of 1.0 will produce a bright blue background.

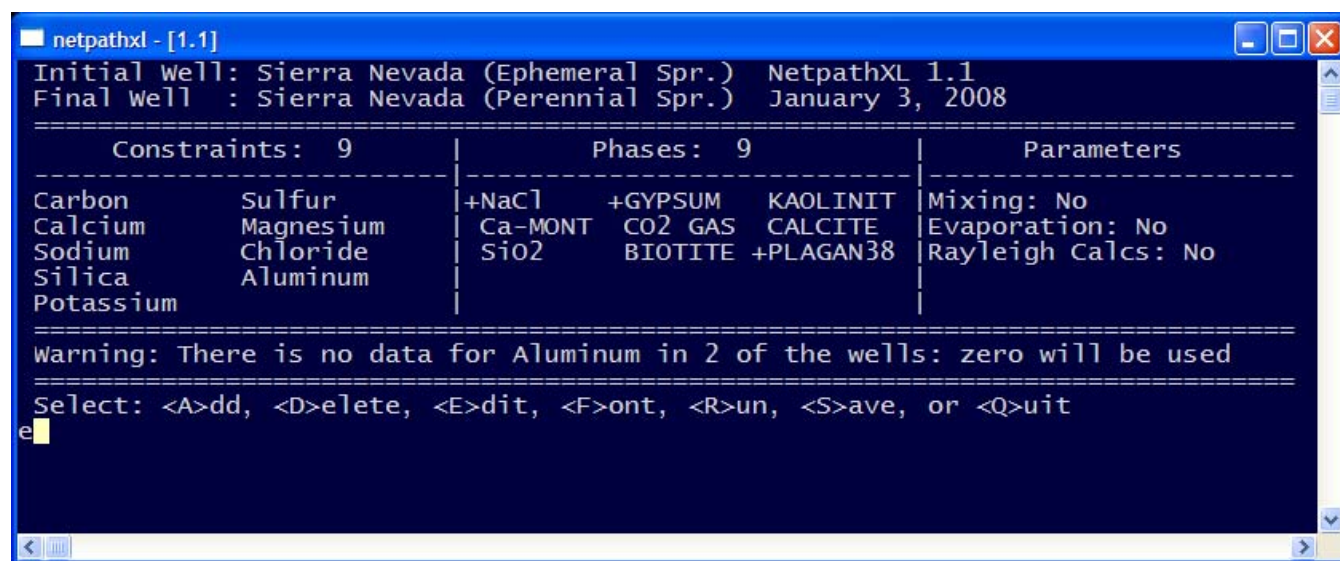


Figure 5. Selecting the edit screen from the main screen of NetpathXL.

Summary and Conclusions

NETPATH is unique in the capabilities it provides for geochemical inverse modeling and radiocarbon dating of ground waters. NetpathXL is a partial modernization of the program NETPATH. NetpathXL simplifies data input by using a fixed-format Excel spreadsheet in place of the program DB. File browsing, installation, and concentration data input have the look and feel of current computer programs. The model-development process remains essentially unchanged from that of NETPATH and requires keyboard input rather than point and click technology. However, keyboard input is efficient and the model development process is simple and straightforward. The calculation engine in NetpathXL is identical to NETPATH.

New capabilities have been added to allow the interchange of data from NetpathXL to PHREEQC and from PHREEQC to NetpathXL. DBXL can translate a NetpathXL spreadsheet file to PHREEQC format (*.pqi*). PHREEQC can translate solution compositions to a NetpathXL *.lon* file. In addition, each inverse model derived by PHREEQC can be written to NetpathXL *.pat* and model files, which allows the PHREEQC inverse model to be reproduced in NetpathXL.

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Plummer, L.N., Prestemon, E.C., and Parkhurst, D.L., 1994, An interactive code (NETPATH) for modeling NET geochemical reactions along a flow PATH, version 2.0: U.S. Geological Survey Water-Resources Investigations Report 94-4169, 130 p.
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Appendix 1. Coding methods

NetpathXL is written in FORTRAN 90 and compiled with Intel[®] FORTRAN compiler within the Microsoft Visual Studio[®] 8.0 programming environment. Originally, NetpathXL and DBXL were written to eliminate the method of screen painting that is used in NETPATH. NETPATH relies on a terminal mode described by *ansi.sys*, which is increasingly difficult to implement in recent Windows[®] operating systems. NetpathXL replaces the routines that cleared the screen and moved the cursor position (*clpart*, *moverelative*, *cls*, *home*, *poscur*) with new routines that use subroutines available for Intel FORTRAN QuickWin Applications, thereby eliminating the use of *ansi.sys*.

With the use of Intel FORTRAN, it was also possible to implement file browsing with standard Windows system calls, which gives NetpathXL and DBXL more of the look and feel of current programming and simplifies the application of these programs in multiple directories.

Finally, the Excel Component Object Module (COM) interface was accessible through Intel FORTRAN and it was possible to replace the functions of DB with Excel. A fixed format spreadsheet was devised for entering the data that were formerly entered through DB. Data entry is much simpler through a spreadsheet and spreadsheet manipulations are familiar to most users. The use of Excel obviates the need for DB although DBXL is used to generate the fixed format spreadsheet and to translate solution data written by PHREEQC.

Appendix 2. NetpathXL Spreadsheet File

NetpathXL requires an Excel file with a specified format. Cell A1 must contain the string “Netpath Spreadsheet 2.14.” Cells A7–AU7 must contain the literal headings specified in table 1. In files generated by DBXL, the cells A1–AU7 are locked so that they cannot be edited. The maximum number of analyses is limited to 400, compared to the limit of 50 in DB and NETPATH. Only rows 8 through 407 may contain analyses. Rows of analyses need not be contiguous; a non-empty well name is required in column 2 for a row to be considered a valid chemical analysis.

If data for an analysis are given in milligrams per liter (mg/L) or parts per million (ppm), then a gram formula weight is used to convert from mass to moles. The default gram formula weights for analytes are given in column 3 of table 1, and, for the case of alkalinity, in footnote 5 of table 1. These gram formula weights are specified in the file *db.dat*. The conversion factor from equivalents of CaCO_3 to equivalents of HCO_3 (1.2193) is hard coded in the source for NetpathXL.

Table 1. Description of cells in a NetpathXL spreadsheet file

Cell number	Required heading	Default gram formula weight in db.dat grams per mole	Meaning of data values	Footnote
A7	Number		Well identification number	
B7	Well name		Well identifier (character string)	
C7	(required)		Options for concentration units	1
D7	Units Flag		Options for interpretation of Eh	2
E7	Eh Flag		Flag for interpretation of carbon data	3
F7	Alk/		Flag for activity coefficient selection	4
G7	TDIC Flag		Temperature, Celsius	
H7	Temp		pH, standard units	
I7	pH		Eh, in volts	
J7	Eh	40.08	Calcium concentration	
K7	Ca	24.312	Magnesium concentration	
L7	Mg	22.9898	Sodium concentration	
M7	Na	39.102	Potassium concentration	
N7	K	35.453	Chloride concentration	
O7	Cl	96.0616	Sulfate concentration	
P7	SO4 as SO4		Alkalinity or total dissolved inorganic carbon concentration	5
Q7	Alk/TDIC	61.0173 or 50.04289	Iron concentration	
R7	Fe	55.847	Manganese concentration	
S7	Mn	54.938	Aluminum concentration	
T7	Al	26.9815	Fluoride concentration	
U7	F	18.9984	Silica concentration	
V7	Si as SiO2	60.0848	Bromide concentration	
W7	Br	79.904	Boron concentration	
X7	B	10.81	Barium concentration	
Y7	Ba	137.34	Lithium concentration	
Z7	Li	6.939	Strontium concentration	
AA7	Sr	87.62	Nitrate concentration	
AB 7	NO3 as N	14.0067	Ammonium concentration	
AC7	NH4 as N	14.0067	Phosphorus concentration	
AD7	P	30.9738	Dissolved oxygen concentration	
AE7	O2(aq) as O2	31.9988	Dissolved sulfide concentration	
AF7	H2S(aq) as S	32.06	Dissolved nitrogen concentration	
AG7	N2(aq) as N	14.0067	Dissolved methane concentration	
AH7	CH4(aq) as CH4	16.0428	Dissolved organic carbon concentration	
AI7	DOC as C	12.011	Redox state of dissolved organic carbon	
AJ7	RS of DOC		Carbon-13 ratio, permil	
AK7	C-13 TDIC		Carbon-14 concentration, percent modern carbon	
AL7	C-14 TDIC		Sulfur-34 ratio of sulfate, permil	
AM7	S-34 SO4		Sulfur-34 ratio of sulfide, permil	
AN7	S-34 H2S		Hydrogen-2 ratio, permil	
	H-2			

Table 1. Description of cells in a NetpathXL spreadsheet file (Continued)

Cell number	Required heading	Default gram formula weight in db.dat grams per mole	Meaning of data values	Footnote
AO7	H-3		Tritium concentration, tritium units	
AP7	O-18		Oxygen-18 ratio, permil	
AQ7	Sr-87		Strontium -87 ratio	
AR7	N-15 N2(aq)		Nitrogen-15 ratio of dissolved nitrogen, permil	
AS7	N-15 NO3		Nitrogen-15 ratio of nitrate, permil	
AT7	N-15 NH4		Nitrogen-15 ratio of ammonium, permil	
AU7	Density		Density, grams per centimeter cubed	

¹ Options for concentration units: 0 millimoles per liter; 1 milliequivalents per liter; 2

milligrams per liter; 3 parts per million; and 4 millimoles per kilogram water.

² Options for calculating the Eh used to speciate redox elements (Fe and Mn): 0 redox is ignored; 1 specified Eh is used; 2 dissolved oxygen is used to calculate Eh; 3 the Sato relation is used to calculate Eh from dissolved oxygen concentration; and 4 sulfate and sulfide concentrations are used to calculate Eh.

³ Options for alkalinity and total dissolved inorganic carbon (Alk/TDIC) data: 0 field alkalinity is entered as HCO₃; 1 carbonate alkalinity (exclusive of all other alkalinity species) is entered as HCO₃; 2 total dissolved inorganic carbon (TDIC) is entered as HCO₃; and 3 field alkalinity is entered as CaCO₃. Note that the gram equivalent weights for the formulas HCO₃ and CaCO₃ are needed only for converting mass concentration units—mg/L (milligrams per liter) and ppm (parts per million)—to moles or equivalents per kilogram water.

⁴ Options for activity coefficients: 0 use the extended Debye-Hückel formula; and 1 use the Davies formula.

⁵ Gram formula or equivalent weights for carbon and alkalinity: for TDIC, the gram formula weight used to convert mg/L and ppm to mol/kg water is 61.0173; for alkalinity, the gram equivalent

weights used to convert mg/L and ppm to equivalents per kilogram of water are 61.0173 for HCO_3 and 50.04289 for CaCO_3 .

Appendix 3. Interfacing with PHREEQC

DBXL can be used to translate analytical data from a NetpathXL spreadsheet (.xls) into a PHREEQC input file (.pqi). Translation is invoked by the fourth option of the options screen for DBXL [“(4) Create PHREEQC input file (.pqi) from NetpathXL file.”]. The root name of the .xls file is the file name, less the .xls extension. The new PHREEQC input file will be named with the root name plus a .pqi extension and will be located in the same directory in which the .xls file resides. The PHREEQC file will be a single **SOLUTION_SPREAD** data block with a row for each analysis in the NetpathXL spreadsheet.

PHREEQC and PhreeqcI versions 2.15 have new capabilities to translate data and inverse models from PHREEQC formats to NetpathXL formats. The “-lon_netpath root” identifier of the **INVERSE_MODELING** data block will write a file named *root.lon* (DBXL .lon format) that contains an entry for each solution composition that has been defined previous to the **INVERSE_MODELING** data block in the PHREEQC input file, including solutions defined by **SOLUTION**, **SOLUTION_SPREAD**, and **SAVE**. The units of the analyses in the .lon file will be millimoles per kilogram water, which may differ from the units with which the solution data were originally defined in PHREEQC. The .lon file can be converted to a NetpathXL spreadsheet with DBXL.

The “-pat_netpath root” identifier of the **INVERSE_MODELING** data block will write a NetpathXL .pat file and multiple NetpathXL model files, one model file for each model found by PHREEQC inverse modeling. Because PHREEQC adjusts concentrations of solutions as part of the inverse-modeling calculation, the adjusted concentrations of a solution may be slightly different for each model that includes that solution. Model-specific solution compositions are written to the .pat file for each inverse model. These adjusted solutions combined with the constraints and reactive phases saved in the model file can be used in NetpathXL to reproduce the PHREEQC model. The solutions in the .pat

file are identified by model number at the beginning of the solution description (Well name). The model number corresponds with the name of the associated model file (*root-n.mod*, where *n* is the model number).

PHREEQC can produce models with fewer phases than constraints, whereas NetpathXL requires an equal number of phases and constraints for each model. It may be necessary to include additional phases in the NetpathXL model definition to be able to reproduce the PHREEQC model. However, the mole transfers of the additional phases in the NetpathXL model should be near zero (roundoff errors may lead to slightly nonzero mole transfers for the added phases). In addition, the definitions of the model file may not be complete in terms of isotope calculations. Any definitions missing from the model that is read by NetpathXL will have to be added through the NetpathXL data-entry screens.