NETPATH-WIN: An Interactive User Version of NETPATH, a Geochemical and Isotopic Mass-Balance Model

Aly I. El-Kadi[a, *], L. Niel Plummer[b] and Pradeep Aggarwal[c]

[a]*Department of Geology and Geophysics and Water Resources Research Center, University of Hawaii at Manoa, Honolulu, Hawaii, USA*
[b]*United States Geological Survey, Reston, Virginia, USA*
[c]*International Atomic Energy Agency, Vienna, Austria*

1. Introduction

The computer program NETPATH (Plummer et al., 1994) is frequently used to construct quantitative models of the chemical evolution of waters along real or hypothetical flow paths in aquifers or other hydrologic systems using hydrochemical data. These models provide important information on geochemical processes and water-rock reactions that can be used to place constraints on numerical models of ground-water flow (Sanford et al., 2004).

NETPATH has been used to investigate geochemical and isotopic reactions in a large number of hydrologic systems for more than 20 years (see for example—Noseck et al., 2009; Lu et al., 2008; Toth and Katz, 2006; Cronin et al., 2005; Plummer and Sprinkle, 2001; Malcolm and Soulsby, 2001; O'Brien et al., 1997; Aravena et al., 1995; Plummer et al., 1990). 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 and software contributions (see for example-- Parkhurst et al. 1982; Plummer et al., 1983; Plummer et al., 1994; Parkhurst, 1997; Glynn and Plummer, 2005).

One of the more important applications of NETPATH is in adjustment of carbon-14 data in initial waters for water-rock reactions in groundwater systems, resulting in a quantitative approach to radiocarbon dating of dissolved carbon in groundwater. The radiocarbon dating analysis of NETPATH utilizes data on total dissolved carbon (dissolved inorganic carbon, DIC; dissolved organic carbon, DOC; and dissolved methane, CH_4). Previous approaches to radiocarbon dating only account for inorganic carbon and a somewhat limited number of reaction possibilities (see for example Ingerson and Pearson, 1964; Fontes and Garnier, 1979; Fontes, 1990; Kalin, 1999). NETPATH is unique among geochemical modeling codes in its handling of radiocarbon dating, utilizing total dissolved carbon, inverse geochemical modeling, and Rayleigh distillation equations (Wigley et al., 1978).

The use of NETPATH involves an iterative approach that requires multiple runs with varying initial conditions and constraints. Originally, NETPATH and an associated database program, DB, were written in FORTRAN 77 for operation in a DOS environment. Recently the data-handling functions of NETPATH were replaced with a new version, NetpathXL that uses Microsoft Excel® (Parkhurst and Charlton, 2008) for data entry. NetpathXL is otherwise identical to NETPATH, and runs in a DOS environment. Although NetpathXL has made it easier to use NETPATH in today's computing environment, the lack of a graphical user interface has limited the use of this software in general. NETPATH-WIN has therefore been constructed to migrate NETPATH applications into the Microsoft WINDOWS® environment.

* Corresponding author. Tel./fax: +8089566331/8089565512. E-mail address: elkadi@hawaii.edu

2. Features of NETPATH-WIN and DB-WIN

The purpose of the graphical user interface for NETPATH is to facilitate data entry and interactive use of the code for testing and accepting various model results. Detailed model-use procedures, description of input variables and terms, and test cases are documented in the original NETPATH report (Plummer et al, 1994), which is included in the NETPATH-WIN package. Two complete data sets are included with the NETPATH-WIN distribution package—1. Test cases associated with the original NETPATH (Plummer et al., 1994), and 2. geochemical models with radiocarbon dating from a study by Plummer and Sprinkle (2001). The user should be familiar with the model, its limitations and assumptions, and data requirements.

2.1. DB-WIN

DB-WIN is an interface for the database program DB (Plummer et al., 1994) that allows entering and editing of chemical and isotopic data for a set of water analyses. DB-WIN permits entry, storage, and editing of up to 50 analyses of water samples for a single file (*file*.lon); calculates mineral saturation indices; and creates the input file (*file*.pat) to be used for constructing reaction models in NETPATH-WIN. All of the features of the original DB program (Plummer et al., 1994) are retained in DB-WIN. New in DB-WIN is the ability to import and/or export data to/from Microsoft Excel® spreadsheets using the CSV format. Previously constructed datasets from earlier DOS applications can be read by DB-WIN, and if desired, exported to Microsoft Excel® spreadsheets. DB-WIN documentation can be accessed through an interactive Instruction tab from the main screen of DB-WIN.

2.2. NETPATH-WIN

NETPATH-WIN is the interface for NETPATH (Plummer et al., 1994), which, given a set of chemical and isotopic constraints, finds all the geochemical mass-balance models that could account for the chemical evolution of one water composition to another for a given set of possible reactant minerals and gases. All of the original features of NETPATH are retained in NETPATH-WIN. Documentation is provided through an Instruction tab from the main screen of NETPATH-WIN. Some of the modeling features of NETPATH include: 1. possible mixing of up to five initial waters with or without further geochemical reaction, 2. inclusion of oxidation-reduction reactions, 3. treatment of the total dissolved carbon system (DIC-DOC-CH_4), and 4. isotopic evolution (N_2, S, Sr, and C) including radiocarbon dating.

3. Software Availability

NETPATH-WIN is maintained by the Isotope Hydrology Section of the International Atomic Energy Agency and can be downloaded free of charge from URL http://www-naweb.iaea.org/napc/ih/index.html, or from the U.S. Geological Survey at http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/netpath/.

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