

United States Department of the Interior

U. S. GEOLOGICAL SURVEY

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Denver Federal Center

Denver, Colorado 80225

September 15, 2010

MEMORANDUM

To: Chief, BRRCR, Lakewood, CO

From: David Parkhurst, BRRCR,, Lakewood, CO

Subject: Transmittal for Director’s approval of “Description of input and examples for PHREEQC version 3—A computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations”, by Parkhurst and Appelo

I am submitting the subject report for publication in a web-only USGS-series report, either a Techniques and Methods (TM) or an Open-File report. I think the report is suitable as a TM report, but I would choose the Open-File format if it allows the report to be released more promptly.

PHREEQC is the most widely used geochemical model in the world and has a mailing list of nearly 1,000 users. Its graphical user interface has been downloaded over 40,000 times. I believe the new capabilities documented in this manual will be widely used and will expand the application of the model. PHREEQC is used to teach basic geochemistry, to simulate laboratory experiments, to investigate natural and contaminated groundwater systems, and to simulate industrial processes. It is used in studies of many of our current environmental issues—radioactive waste disposal, natural remediation of inorganic and organic contamination, and acid mine drainage. The new high-pressure capabilities of the model are particularly useful for investigation of carbon dioxide sequestration.

The report documents the current capabilities of the geochemical reaction model PHREEQC. Version 2 of PHREEQC was published in 1999 (Parkhurst and Appelo) and many capabilities have been added in the intervening decade, which are now fully documented in this report.

The report has been written in FrameMaker because it was possible to build on the documentation of PHREEQC version 2. The FrameMaker document can be used to produce a PDF file, which has extensive links to enable easy navigation in the PDF document. It is not possible to translate the report into Word easily, and it is not likely that the links and equations could be reproduced. So, I request that the editorial review be done with the PDF file and that I format the final PDF for web distribution. This approach worked effectively for the publication of TM6-A35 (reactive-transport model PHAST).

The subject manuscript has been through colleague review by Ray Johnson (USGS), David Kinniburgh (British Geological Survey), Rasmus Jakobsen (Danish Technical Institute), and Luc van Loon (Maastrict University, Netherlands; example 21 only). I have responded to the reviews of Johnson and Kinniburgh and my coauthor has incorporporated changes in response to the reviews of Jakobsen and van Loon. I believe the reviews and our responses have been comprehensive and the report is ready for final editorial review and final approval.