REVIEW OF THE MARCH 1, 2005 DRAFT RESEARCH REPORT ENTITLED "DOCUMENTATION AND APPLICATION OF THE REACTIVE GEOCHEMICAL TRANSPORT MODEL RATEQ"

I. Review Scope

Reviewers provided preliminary comments on a December 1, 2004 [1] version of the subject report. Subsequently, an updated version of the report, dated March 1, 2005 [2], was provided to the reviewers. The March 1, 2005 version of the document incorporates many of the suggestions made by the reviewers based on the December 1, 2005 version of the document. Comments in this document pertain to the more recent version of the report [2].

Comments are based on a review of the reports as well as trial runs of the RATEQ code. Trial runs were made using example files that were sent to the reviewers by the author. During the trial runs, input values of the example problems were perturbed and the corresponding changes in the outputs were noted. The purpose of these exercises was not to evaluate the performance of the RATEQ code, but to evaluate the usefulness of the manual to the reviewers in conducting these exercises and understanding the code output.

II. General Comments

1) Because of the complexity of the physical systems modeled by RATEQ, creation of appropriate models will require input from persons expert in developing hydrologic as well as chemical models. This requirement is inherent to the complex problems that RATEQ can be used to model and is not a shortcoming of the documentation. However, the high level of both chemical and hydrologic expertise required to use the code effectively may limit its use if guidance is not provided with the code. Although outside the scope of the reviewed documents, use of the code would be facilitated by additional documentation that describes the physical meaning of parameters used in the code and gives additional guidance on probable ranges of those parameters.

2) The manual focuses on the format of the input files. In addition to the format of the input files, it would be helpful for the manual to include instructions on running the code. The March 1, 2005 [2] version of the report includes an improved description of the relationship between MODFLOW-2000 [3], MT3DMS [4], and RATEQ, which is expected to be helpful to the user. However, it is expected that the non-expert user would benefit from instruction on running the codes from the command line and requirements for interfacing MODFLOW and RATEQ. For example, it would be helpful for the manual to include a discussion of topics such as changing environment variables to include MODFLOW and RATEQ in the user's PATH and the preferred directory structure to use with MODFLOW and RATEQ executables and input files.

3) The example files provided to the reviewers demonstrate different setups for RATEQ problems, and it is suggested that they be made available with the code. The manual could be further enhanced by a section that briefly discusses the purpose of the files associated with each problem. Although the purposes of the RATEQ input packages are summarized in Table 3.3 [2] and discussed in the text, the example problems include files that do not appear to be RATEQ input packages. For example, the example problems include several files with the

extension “rtq”. The purpose of these files is unclear because the NAM files in the example problems do not include these files.

4) Section 5.3 of the manual [2] briefly mentions that the MODFLOW files for one of the example problems were created with the Argus [5] graphical user interface for MODFLOW. It would be helpful for the manual to include a discussion of whether the Argus user interface is available to the public, and whether RATEQ can run with MODFLOW output files created by other programs that include a graphical user interface for MODFLOW (e.g., Groundwater Vistas or the Army Corps of Engineers’ Groundwater Modeling System). In addition, because RATEQ uses some files that MT3DMS also uses, it would be helpful to include a discussion of whether RATEQ can run with files created by a program that includes a graphical user interface for MT3DMS.

5) It would be helpful for the manual to include guidance on using the results of the output files. Section 1.1.2 [2] indicates that custom Matlab scripts are distributed with RATEQ that allow the user to view breakthrough curves and concentration snapshots, but no explanation is provided of how to use the scripts. Annotated examples of output files and instructions regarding use of the Matlab scripts distributed with RATEQ would facilitate use of the code.

6) It would be helpful for example problems to contain references to pages in the manual that explain the keyword or option being used. It was necessary to refer back to the text to understand the example problems, especially because the arguments of many of the options were not labeled in comments in the files.

7) There appear to be opportunities for error caused by the use of incorrect units because the program does not read units from many types of input data. For example, in the example problem in Table 5.1 [2], the duration of a flow interruption is specified as 4.17 (without units) and it is explained in the caption of Figure 5.1 that the duration of the timed event was 4.17 hours [2, p. 74]; however, in the same example problem the maximum time of the simulation is specified as 6.5 days, and the velocity is specified in units of m/yr. It is unclear where the units of the timed event are specified, and why they are different from the time units of the maximum time of the simulation. Because RATEQ does not convert units automatically, the use of different time units in the same simulation is potentially confusing to the user, especially when it is unclear where in the input file the units of the timed events are specified. The optional variable Time-units, which can be included in the definition of kinetic reactions and is checked for consistency with the time units used in the Basic Transport (BTN) file [2, p.39], is expected to be very helpful to the user, especially if an appropriate error message is generated when a run is stopped due to a mismatch between the time units of the kinetic constant and the time units used in the BTN package.

III. Specific Technical Comments

1) The term Geochemical Reaction (GCR) package used in the December 1, 2004 version of the manual appears to have been replaced with the term Geochemical Solver (GSR) package in the March 1, 2005 version of the manual [2]. However, the name (NAM) files in the example problems provided to the reviewers did not include any references to GSR files, and instead contained references to GCR files. This potentially confusing inconsistency should be corrected if the example files will be released to the public. In addition, although the meanings

of package abbreviations are included in the text on pages 19 and 20 [2], it would be helpful if Table 3.3 [2] included the abbreviation for each type of input package as well.

2) The NAM files for the example problems provided to the reviewers do not contain any references to RDB files, which is unexpected because the manual recommends the use of RDB files [2, Table 3.3].

3) MT3DMS was provided to the reviewers with the example problems. It is unclear whether it was provided as a courtesy, or whether MT3DMS must be present for RATEQ to run.

4) Equations in Chapter 2 and Appendix 1 should be reviewed for the consistency of subscripts and inclusion of variable definitions. For example, in Equation 2-8 [2] the porosity values appear to be missing subscripts and the dirac delta function is written with a superscript in the equation but defined with a subscript. The clarity of Appendix 1 would be improved if definitions of all of the variables used in the appendix were provided in the appendix.

5) If the Array Reader package, which is described as a necessary input package for MT3DMS in Section 3.3.2 [2], is also a necessary input package for RATEQ, it is unclear why it is not included in the summary of required input packages in Table 3.3 [2].

6) The discussion of the Array Reader input file in Section 3.3.2 indicates that the possible values of the argument “input_option” are “const”, “file” and “next” [2, p. 23]. However, the meaning of the value “next” is not explained in the text.

7) The input for the NCOMP and SRCONC parameters in the BTN file require additional explanation [2, p. 26]. The text indicates what the value of the parameter SRCONC should be if NCOMP equals one, but does not indicate what the value of SRCONC should be if NCOMP is greater than one. The summary of the format of the BTN package in Table 3.7 [2] does not include the parameter SRCONC, and it is, consequently, unclear where this parameter should be included in the BTN package file. The relationship between the parameters SRCONC and SCONC is unclear.

8) Text in the description of Record 15 of Table 3.7 [2, p.27] indicates that “the codes for print-formats are the same as those listed in Table 3.7". The meaning of this statement is unclear because print formats are not described in Table 3.7.

9) The meaning of the “guess” parameter in the GSR package should be further clarified. The manual states only that “guess is an optional value that is used as an initial guess in computing the speciation” [2, p. 45] but does not indicate what forms of the element the guessed value includes. The meaning is difficult to infer from the example problems. For instance, the example in Table 6.1 lists UO_2^{+2} as an aqueous species with a concentration of 4.0 E-6 M and an initial guess of 1 E-24 M. This entry appears to indicate that the concentration of dissolved uranium is 4.0 E-6 M, of which 1.0 E-24 M is in the UO_2^{+2} form. However, in the same example, Br^- is listed as an aqueous species with a concentration of 1.0 E-5 M, and an initial guess of 2.0 E-3 M. One might assume, by analogy with the entry for uranium, that the aqueous concentration of Br is 1.0 E-5 M, of which 2.0 E-3 M is in the Br^- form. However, because the value of the “guess” parameter is two orders of magnitude greater than the aqueous concentration of Br , it appears that the initial guess also includes sorbed or precipitated species.

10) The option force_rate is included in Tables 5.1 and 6.3 [2] but is not discussed in the text. It is unclear why this option would be used because the default behavior described in the text [2, p. 37] is that a rate is always used if a rate controlled equation is included in the input file and the equilibrium relationship is used if a rate is not given.

11) In the example in Table 5.1 [2], species to be ignored are listed both in Reaction Set 1 and in the Calculation Block. Because the Calculation Block specifies that Reaction Set 1 is to be used in the transport equations, it is unclear why the species to be ignored must be listed again in the Calculation block. An explanation of this requirement would be helpful to the user.

12) Several of the tables that contain example files in Chapters 4, 5, and 6 have captions that indicate simply that the table presents a "RATEQ input file". Captions that indicate which type of file is presented in the table would be more helpful to the user.

IV. Clarifying Comments

1) The March 1, 2005 version of the report [2] would benefit from an editorial revision. For example, the last two paragraphs on page 21 [2] are repeated exactly at the beginning of page 22. A sentence in Section 1.1.1 [2] begins "The second additional file species the composition of each of various solutions...", the meaning of which is unclear. Several sentences seem to lack final punctuation (e.g., the last sentence of Appendix I, the last sentence before Section 3.3.1, and the penultimate sentence on page 29, among others). The first paragraph on page 27 terminates with a closing parenthesis, but no matching opening parenthesis is apparent. Table numbering formats are inconsistent (c.f., Table 3-1. [2, p.18] and Table 3.2 [2, p.18]). In addition, the document does not appear to have a page numbered 97, and skips from page 96 to page 98. Because this list is merely illustrative and not exhaustive, it is suggested that the document be reviewed by a technical editor prior to publication.

2) Section 1.1.1 [2] indicates that RATEQ requires two input files that are not required by MT3DMS. The sentences that follow describe "The first file...", "The second additional file...", and "Finally, the last new input file...". Thus it is unclear whether RATEQ requires two or three input files that are not required by MT3DMS.

3) The package type "DSP" is not included in the list of possible package names in the text [2, p.19]. This package type is expected to be included in the list because it described as an input package type in the following paragraph [2, p.20].

4) The discussion of Array Reader package input values in Section 3.3.2 includes two sentences in different places that describe the meaning of a value of zero for the parameter IREAD. The first indicates "If IREAD = 0, every element in array will be set equal to the value CNSTNT" [2, p.21]. The second indicates "If IREAD=0, every element in the array is set equal to CNSTNT/ICONST" [2, p.22]. It is unclear why the description is given twice, and it is unclear why one instance indicates the array elements will be set to a value of CNSTNT and one indicates the array elements will be set to a value of CNSTNT/ICONST.

5) The logical meaning of the outline designation "b" at the top of the second column of text on page 22 [2] is unclear, because the section does not contain the outline designation "a".

6) Table 3.7 [2] is missing information in the third column of rows 14, 15, and 17-23. Similarly, Table 3.1 [2] is missing information in the third column of the rows describing the Well and Hydrogeologic Unit Flow MODFLOW packages.

7) The numbering of records in Table 3.12 [2] appears to be inconsistent with the numbering of records in the discussion of the table in the text. In particular, the numbering of records 13, 14a, and 14b should be clarified. Similarly, Table 3.18 [2] includes a record 14, which is omitted in the discussion of the table in the text.

V. References

1. Curtis, G.P., "Documentation and Application of the Reactive Geochemical Transport Model RATEQ". December 1, 2004.

2. Curtis, G.P., "Documentation and Application of the Reactive Geochemical Transport Model RATEQ". March 1, 2005.

3. Harbaugh, A.W., Banta, E.R., Hill, M.C., McDonald, M.G. (2000) MODFLOW-2000, The U.S. Geological Survey Modular Ground-Water Model - User guide to Modularization Concepts and the Ground-Water Flow Process. Open-File Report 00-92. U.S. Geological Survey, Restin, Virginia.

4. Zheng, C., Wang, P.P., (1999) MT3DMS: A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems; Documentation and User's Guide. U.S. Army Corps of Engineers, Engineer Research and Development Center. Contract Report SERDP-99-1.

5. Winston, R.B., (2000) Graphical User Interface for MODFLOW, Version 4: U.S. Geological Survey Open-File Report 00-315.