# 1 INTRODUCTION

## 1.1 Overview

This chapter provides an overview of the MOUSER software. MOUSER implements solutions to the one-dimensional advective-dispersive-reactive (ADR) equation for a variety of boundary conditions and reaction scenarios. Although MOUSER was originally developed to simulate subsurface barrier systems (slurry walls and permeable reactive barriers), it is applicable to any problem defined by the one-dimensional ADR equation, including advection- or diffusion-dominated laboratory columns and field-scale transport along a streamline. General information about the computer program is presented here in Chapter 1. Chapter 2 presents the governing equations solved by the models. Chapter 3 includes detailed instructions for the preparation of input files. Chapter 4 includes a general discussion of ADR modeling and parameter selection for a variety of applications. Chapter 5 provides an overview of example problems that can be downloaded from the MOUSER web site. The remainder of the manual (Chapters 6-11 and Appendices) is devoted to details of the numerical implementation of the ADR solutions and programming issues, and portions are currently available only on request.

## 1.2 Unique features

MOUSER contains some features that are similar to other public domain one-dimensional ADR codes such as CXTFIT (Parker and van Genuchten, 1984) and PHREEQC (Parkhurst and Appolina, 2000), but emphasizes the following distinctives:

- Three alternative solution methods are available: (1) analytical (closed form), (2) semi-analytical, based on the numerical inversion of Laplace-transformed solutions, and (3) numerical, using several algorithms built around a flexible grid-based split-operator approach.
- Numerous boundary condition options are provided for both the domain entrance and exit.
- In addition to the solute concentrations(s), the program can provide output for the following derived variables: instantaneous flux per area, cumulative mass per area, sorbed concentration, and total (aqueous plus sorbed) concentration.
- A variety of reaction options are supported, including nonequilbirum sorption, sequential multi-solute parent-daughter decay, and multi-solute competitive cation exchange. Extension to new reaction systems is ongoing.
- Instructions are available for modeling customized reaction scenarios by developing FORTRAN source code compatible with the other MOUSER modules (currently by request only).

## 1.3 Input and output

MOUSER solves the governing ADR equation for a two-compartment system consisting of an immobile solid phase (porous media) and a mobile pore fluid phase. The required input parameters for MOUSER include information regarding physical and chemical properties of the contaminant(s) and porous media. Preparation of input is readily accomplished using a text editor. Detailed discussions of the required input parameters are contained in Chapter 3, with general application-specific guidance for parameter specification provided in Chapter 4.

The MOUSER output consists of calculated values of the contaminant(s) aqueous concentration, instantaneous flux and cumulative mass released per area, and/or sorbed/total concentrations The output is written in space-delimited ASCII format to a text file, which may be easily imported into a spreadsheet or graphing program. Output is provided for the dependent variables in terms of a temporal profile (time-varying output for a specified location) or a spatial profile (output for multiple spatial locations at a single time).

The contaminant *aqueous concentration* ($ML^{-3}$) is expressed as a *volume-averaged* (i.e., resident) concentration in terms of mass of aqueous solute per volume of pore fluid, although interpretation as a flux-averaged concentration is possible under some circumstances. The *instantaneous contaminant flux* ($MT^{-1}A^{-2}$) is defined as the rate of contaminant mass exiting a plane normal to the direction of advective transport, expressed in units of solute mass per cross-sectional area per time. *The cumulative mass per area* ($MA^{-2)}$ is simply the summation of the total mass of contaminant released from the domain during the simulation period, with units of mass per cross-sectional area (normal to direction of advection). When applicable, the *sorbed concentration* is expressed as the mass of sorbed solute per mass of solid material, and the *total concentration* (includes pore fluid) is expressed as the combined mass of solute in the aqueous and sorbed phases per mass of solid material.

## 1.3 Installation and use

The MOUSER executable program can be downloaded from www.groundwater.buffalo.edu and copied into the desired Windows folder. At the time of this writing, the public domain version of MOUSER has been compiled as a "console application" using the Compaq FORTRAN Developers Studio, Version 6.6. Console applications run in a DOS environment regardless of which version of MS Windows serves as the operating system. Execution is best accomplished by running the "command prompt" from the Windows *Programs* menu, changing to the directory that contains the MOUSER executable and data files, and typing "mouser" at the prompt. The user will then be prompted to enter the name of the primary input file. The program can also be run by mouse-clicking the program icon, but any error or output messages written to the screen will probably pass too quickly to read.

## 1.4 Technical references

MOUSER implements and builds on concepts originally developed for TRANS1D, a model used in research sponsored by DuPont. Discussions of some of the technical issues related to TRANS1D/ MOUSER applications can be found in the following journal articles and conference papers, which are available by request from the authors:

- Rabideau, A. J. (1996). "Contaminant transport modeling," in *Assessment of Barrier Containment Technologies*, Rumer, R.; Mitchell, J., Eds., prepared under the auspices of U. S. Department of Energy, U. S. Environmental Protection Agency, DuPont Company, NTIS PB96-180583, 1996. An overview of modeling issues relevant to barrier technology.
- Khandelwal, A., Rabideau, A. J., and Su. J. (1997). "Development of contaminant transport model for the design of vertical barriers," *Land contamination and reclamation*, 5(3), 97-101, from 1997 *International Containment Technology Conference*. An overview of an early version of the TRANS1D model with application to column experiments performed with soil/bentonite slurry wall materials.
- Khandelwal, A., Rabideau, A. J. (1996). "Modeling of diffusion-dominated transport in soil/bentonite slurry walls," *Proceedings of the twenty-eighth Mid-Atlantic Conference on Hazardous and Industrial Waste*, Buffalo, NY, July 1996. An overview of an early version of TRANS1D, and preliminary results from column experiments.
- Khandelwal, A., Rabideau, A. J., Shen, P. (1998). "Analysis of diffusion and sorption of organic solutes in soil/bentonite barrier walls," *Environmental Science & Technology*, 32(9), 1333-1339. Results and interpretation of selected column experiments performed with organic solutes and soil/bentonite barrier materials.
- Rabideau, A. J., and Khandelwal, A. (1998). "Analysis of nonequilibrium sorption in soil/bentonite barriers," *Journal of Environmental Engineering*, 124(4), 329-335. Derivation of single-solute finite layer model, with discussion of the role of nonequilibrium sorption in soil/bentonite slurry walls.
- Rabideau, A. J., and Khandelwal, A. (1998). "Boundary conditions for modeling transport in vertical barriers," *Journal of Environmental Engineering*, 124(11), 1135-1141. Recommendations for boundary conditions for modeling slurry walls and introduces concept of "mixing zone" conditions.
- Rabideau, A. J., Shen, P., and Khandelwal, A. (1999). "Feasibility of amending slurry walls with zero-valent iron," *Journal of Geoenvironmental and Geotechnical Engineering* 125 (4), 1135-330-334. Analysis the potential performance of soil/bentonite slurry wall materials amended with zero-valent iron.
- Khandelwal, A., and Rabideau, A. J. (1999). "Transport of sequentially decaying reaction products influenced by linear nonequilibrium sorption," *Water Resources Research*. Derivation of multi-solute finite layer model, with discussion of applications to iron-based treatment walls.