Hans-Jörg G. Diersch

FEFLOW

Finite Element Modeling of Flow, Mass and Heat Transport in Porous and Fractured Media

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This book is dedicated to my father, Willy.

Preface

Flow, mass, and heat transport processes in nature and geosphere are highly (if not even most) complex. There is an increasing demand in studying and predicting such kind of problems in an environmental and geohydrodynamic context. This demand naturally results from the growing human influence on the environmental and natural resources with their constraints and consequences. Men are also looking for new technologies of exploiting geothermal energy and storing fluids in reservoirs. Industries are developing new materials with improved properties for which a greater understanding of flow and energy transport is required. Among all of these applications, a very important subclass of processes occurs in structures which are categorized as *porous and fractured media*. Those structures exist in many natural and man-made systems having length scales differing by several orders of magnitude. Lengths range from pore and fracture scales in the order of micrometers and millimeters, textile and tissue materials measuring tens of millimeters, the diameter of wells in the order of tens of centimeters, the thickness of aquifer layers and geologic strata in the order of meters to tens of meters, the distances between wells and thicknesses of aquifer systems with tens to hundreds of meters, and the extent of reservoirs and subsurface fields up to tens or even hundreds of kilometers. Heterogeneities and parameter contrasts have to be encountered in all these length scales.

To understand the processes, to make them predictable and controllable, we need models. Models are abstractions of the real systems. However, abstractions are not to be considered as our resort and insufficiency in finding a description for *all* phenomena and influences. They represent a necessary and appropriate level of reduction and idealization where the (most) important processes are emphasized and the subordinate processes are dropped. This is the way (and obviously the only way) to find causal relationships and to set up predictive tools. We don't need a second perfect copy of nature; we have it already in the form of our experiments and observations made at the real system.

The construction of the model is the first and very important step in a modeling process. It is termed as model *conceptualization* which covers the description of the system's composition, the physical and physicochemical phenomena, and

the relevant properties of the medium in which they occur. Obviously, such a description includes assumptions and simplifications which are subjectively selected by the modeler and, consequently, it reflects his understanding and faculty of the matter in a specific scope of interest. Accordingly, a model as a simplified version of reality is subjective, and nonunique models exist in dependence on the level of assumptions, contexts of intended applications, and the state of knowledge. Fortunately, at present model conceptualization can be based on an advanced and general framework of physics and rational thermodynamics, allowing us to objectify the modeling approach for a large range of applications. However, this requires that the modeler is conversant with these conceptual steps and understands the basic physical/thermodynamic principles of the model in order to, at least, examine the physical background of the model with its assumptions and limitations. Nowadays there is a desire to develop models (family of models) which cover a wide range of applications.

The second step in modeling is the mathematical representation of the conceptual model in the form of numerical schemes and discrete solution techniques. There are many ways to do that. However, for satisfying also the requirements of a wide range of applications as stated above for the conceptual working step, one of the best choices is the *finite element method* (FEM). The FEM is very general and useful for practical applications. Its geometric flexibility and the ability to accurately apply the appropriate boundary conditions on complex domains make the FEM superior to other numerical strategies, such as finite difference methods (FDMs) or finite volume methods (FVMs). The understanding of the actually used spatial and temporal discretization techniques is necessary for modelers who practically solve flow and transport problems and interpret the numerical results with respect to accuracy and reliability of the achieved simulation results.

The third (and final) step of modeling is the computational realization of the model (family of models) in the form of an appropriately developed *simulation software*. The graphical interface of such a simulation code represents the 'working shell' for the modeler dealing with the preparation of the input data and the execution and the evaluation of the computational results of a model. Since the software interface is the only visible and operational part of the modeling process, it can be seductive for a common or novice user to exclusively apply the software as a black box, widely ignoring the theoretical modeling basis. There is indeed a potential danger for an uncritical use of modern software. Here, a graphically very sophisticated computation can create the false impression that the quality of the numerical solution is comparable to the quality of the graphical presentation. (But the reverse of this statement is also not true: A crude graphical presentation does not necessarily indicate proper solutions.)

From the above it becomes obvious that the modeling of flow and transport processes encountered in porous and fractured media has, at least, three important faces: the conceptual, the numerical, and the software/application aspect. An "ideal" modeler should have best knowledge of all of these three subjects. But this book is not primarily addressed to such a type of a "perfect" modeler (if ever it exists), but I think, at least, both the basic concepts and the practical aspects should be reasonably

well known and understood by engineers, applied scientists, and practitioners who use or intend to use models for simulating flow and transport processes in porous and fractured media.

This book is written, on the one hand, for expert modelers in this field to make the theoretical basis more understandable. On the other hand, it is also written for novices and practitioners who make contact with the matter as a software user for the first time and (hopefully) intend to improve their understanding and knowledge of the modeling basis. As the title of the book could indicate, the book is not intended as a user's guide, at least in the common sense, which would mainly emphasize software functionalities and handling. On the other hand, "real" modeling, if going into practice, should necessarily be concrete and the modeler has to decide for a specific software package (sometimes more than one). The software, which is related to this book, is FEFLOW® [125].

FEFLOW is an acronym of *finite element subsurface FLOW simulation system* and solves the governing flow, mass, and heat transport equations in porous and fractured media by a multidimensional FEM for complex geometric and parametric situations including variable fluid density, variable saturation, free surface(s), multispecies reaction kinetics, non-isothermal flow, and multidiffusive (thermohaline) effects. It is capable of handling a wide spectrum of problems ranging from theoretical studies to practical real-site applications. To master all of these supported problem classes and model options, a large degree of experience and detailed information are needed. FEFLOW comprises theoretical work, modeling experience, and simulation practice from a period of about 40 years (Table 1). In this light, the main objective of this book is to share this achieved level of modeling with all required details of the physical and numerical background with the reader. The FEFLOW book is a theoretical textbook and a reference guidance for modeling in one piece – in one hand. The theoretical basis of modeling is thoroughly described but will not stand alone; it becomes really accessible and applicable with FEFLOW. That is what I advocate and actually provide with this book: *modeling that works*.

The book is intended to put advanced theoretical and numerical methods into the hands of modeling practitioners for porous and fractured media. It starts with a more general theory for all relevant flow and transport phenomena on the basis of the continuum approach, systematically develops the basic framework for important classes of problems (e.g., multiphase/multispecies flow and transport phenomena, unsaturated-saturated problems, free-surface groundwater flows, aquifer-averaged equations), introduces finite element techniques for solving the basic 3D and 2D balance equations, in detail discusses advanced numerical algorithms for the resulting nonlinear and linear problems (e.g., adaptive techniques, variable switching strategy, upwinding schemes), and completes with a number of benchmarks, applications, and exercises to illustrate the different types of problems and ways to tackle them successfully (e.g., flow and seepage problems, unsaturated-saturated flow, advective-diffusion transport, saltwater intrusion, geothermal and thermohaline flow). All examples can be rerun, modified, and extended by using FEFLOW.

The chapters of the book can formally be grouped into two major parts: physical basis and numerical basis with benchmarks and applications. The book is not meant

Table 1 Major historical stages of FEFLOW development

Year/period	Issue
1979	*Birth* and first manifestation [128] based on the finite element predecessor program FINEL developed since 1973 [126, 127, 142]
1979–1986	*Version 1.* FORTRAN research-oriented batch program; implementations for mainframes IBM 370, EC 1055, BESM-6 with punch card input and hardcopy printed output; limited pre- and postprocessing; FEFLOW already provided an extended finite element library (quadrilaterals and triangles of linear, quadratic, or cubic type) and was able to compute 2D transient groundwater flow and transport problems [129]. Effort in modeling variable-density flow problems was initiated [130, 133]
1987–1990	*Version 2.* First interactive prototype for SUN workstations and ATARI ST microcomputer. The code was completely rewritten from FORTRAN into C. FEFLOW became the first fully interactive and graphics-based finite element simulator in groundwater [134]
1990–1992	*Version 3.* Starting commercial development. X Window System and OSF/Motif GUI implementation, installations on various UNIX graphics workstation platforms (e.g., SGI, SUN, IBM, HP, Sony, DG, DEC). Extension to 3D (1992). FEFLOW became a registered trademark (1992)
1992–2001	*Version 4.* Considerable software extension, among others: thermohaline transport modeling (1993), 3D visualization tools and GIS interfacing (1995), adaptive meshing and data store manager (1996), unsaturated flow modeling (1997), MS Windows 95/NT installation (1997), IFM programming interface (1998), and integration of parameter estimator PEST and nonlinear dispersion (2000). In the extensions of the code object-oriented programming with C++ became increasingly present
2002–2009	*Version 5.* Further advances: discrete feature elements and extended possibilities for unsaturated flow (2002); fast TRIANGLE [475] mesh generator, algebraic multigrid (SAMG) [499] equation solver (2003); multispecies transport, reaction kinetics editor, transient pathline computations, FEFLOW Explorer for 3D visualization and animation (2005); 64-bit technology, variable-density multispecies multidiffusive transport, new mesh generator GRIDBUILDER [369], scatter plots, expression editor for sink/sources (2006); and borehole heat exchanger simulation, spline interpolation, improved parallelization (2008)
2009–2012	*Version 6.* New *Qt*-based graphical interface replaced the classic X11 and OSF/Motif GUI providing a modern and powerful environment for modeling and simulation available for both MS Windows and LINUX operation systems. GUI, data management, and part of the computational finite element kernel were transformed to a rigorous object-oriented architecture based on C++
2012–. . .	*Version 6.1.* Completion of the new object-oriented software architecture with *Qt*-based GUI. 3D sterioscopic graphics available. Improvements in parallel computing and high performance in large data treatment and simulation

to be read from front to back. The first part can also be of interest for those readers who wish to learn more about continuum mechanics for flow and transport phenomena in porous and fractured media. Others could primarily be interested in the finite element method with the embodied numerical algorithms. However, I assume most readers will start up with a software play and will hopefully be more

interested in the basics later on (as the inductive way of learning – “from the surface into the ground”). To support this approach, I endeavor to present the subject in a complete and unified manner. At the beginning of the book, the preliminary chapter will summarize all important notations, definitions, and fundamental algebra used throughout the text.

I hope the book will be useful for both students and practitioners in engineering and geosciences as well as in other fields where porous-media flow dynamics and computational methods are of specific concern. I suppose that the reader already possesses (or approaches) an advanced degree in engineering or applied sciences and has an interest in geohydrodynamic flow modeling. I assume that the reader is somewhat versed in physical/mechanical principles and numerical mathematics.

Berlin, Germany Hans-Jörg G. Diersch
March 2013

Acknowledgments

This book accumulates modeling work over a period which I started in 1973 at the Dresden University of Technology, Germany, with finite elements. In 1979 I began to focus on groundwater and porous-media flow modeling and started the FEFLOW development at the former Institute of Mechanics in Berlin (Academy of Sciences of East Germany). I spent 12 fruitful years at this Academic Institute in computational fluid mechanics, which I deeply acknowledge. In 1990 I founded the WASY company together with partners (in 2007 renamed to DHI-WASY GmbH) in Berlin, Germany, where FEFLOW has been further developed, continuously improved, and extended. Since that time the capabilities of the code have been increased substantially. I thank the FEFLOW developing group at DHI-WASY for their enthusiasm and contributions. With the book I would like to express my gratitude to all previous and current colleagues who are directly or indirectly involved in achieving the success of FEFLOW as a scientific and commercial software. I hope the book can provide a secure and fertile basis which I would like to hand over to the next generation of FEFLOW developers.

My most special appreciation is dedicated to my wife Renate who has accompanied my work since the time when FEFLOW consisted of 500 punched paper cards, ran on a computer bigger than a house, and the only available plotter was my own hand (drawing velocity arrows of about 1,000 nodes!). She is the only one who can really mark the miles I went through the times.

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