

1. INTRODUCTION

This manual presents the basic theories of groundwater flow and contaminant transport as applied to the construction of numerical models. Chapter one discusses some of the practical questions that may be investigated with a numerical model, the capabilities and limitations of such models, a review of the different ways of approximating solutions to groundwater problems and the general procedure for constructing a model.

Important equations that govern groundwater flow and solute transport are reviewed in chapter two. Numerical modelling involves approximation of the equations especially to describe systems that have variable properties and irregular geometry. Analytical solutions are often not available for such systems. Numerical procedures used to describe groundwater problems create systems of equations that must be solved simultaneously. The equations must also be solved efficiently and fairly accurately. Some of the methods widely used to solve simultaneous equations are therefore discussed in chapter three.

Most groundwater models are based on either the finite difference or the finite element formulation. Basic principles of the two methods are discussed in chapters four and five respectively. Examples and case studies are provided for both methods in each chapter while details of the case studies are provided in appendices 1 to 3. Particle tracking methods are presented in chapter six as alternatives to finite difference and finite element methods for the simulation of contaminant transport.

A list of references is provided in chapter seven and a glossary of selected terms is given in chapter eight. Appendix 4 contains a list of some groundwater modelling codes which are based on the formulations presented in this manual.

1.1 Definition and Purpose of Modelling

Models (be they physical, analog or mathematical) are an attempt to represent reality. In groundwater studies, numerical models are often used as tools that help us understand the physical, chemical, and biochemical processes taking place in groundwater systems. They also help us understand the intricate interactions between these processes and provide the information we need in order to manage these processes beneficially, without harm to the environment. Numerical models are now used in virtually all areas of groundwater hydrology.

Groundwater models can be broadly grouped into two categories: water quantity (generally requiring flow models) and water quality (requiring transport models). In the water quantity category, models are used in aquifer management, well field design, recharge enhancement, determination of optimum yield, well interference studies, studies of groundwater-streamflow interactions, and similar problems. Models of this type have been well proven in many years of use.

In the groundwater quality category, numerical models are used to study the consequences of groundwater contamination, the means that are needed to prevent contamination, the design of remediation measures and to test effectiveness of alternative remediation schemes. Specifically, models can shed light on typical questions such as the following:

- what is the migration path of a contaminant in the groundwater?
- will the contaminant reach a specific location of interest, such as a water well?
- if migration to the location occurs, how long will it take?
- how important are attenuation mechanisms such as dilution, dispersion, and chemical or biochemical transformations?
- can the contaminant be removed by a specific remedial action?

- how effective are natural or artificial remediation processes in removing the contaminant?

Numerical models for basic transport processes such as advection-dispersion are also well proven. In more advanced areas (such as flow in variably saturated media, flow in fractured media and the transport of multiple chemically or biochemically interacting substances in a spatially discrete and dynamic framework) some models have been developed and intensive research is continuing.

1.2 Proper and Misuse of Models

Because models are representations of real-world systems, they are generally as good as our understanding of the systems being modelled.

Natural groundwater systems are often highly complex and a complete description of the physical characteristics is in most cases impossible. Instead, the physical properties of the system are generally described either in terms of averages or in the form of statistical distributions. Also, physical/chemical/biochemical processes can interact in complex ways and some of these interactions (i.e. reaction kinetics) are not yet fully understood.

In view of these complexities, the use of models in a purely predictive-deterministic mode is risky and generally justified only in simple situations. Groundwater models are properly used for purposes of, for example:

- obtaining insight into complex processes,
- assessing the relative importance of the various processes occurring in a given situation by means of sensitivity analyses,
- analyzing "worst-case", "special case" or "what if" situations,

- making probabilistic predictions.

Models also play a vital role in research into the behaviour of hazardous contaminants in the subsurface. For example, large-scale field experiments involving chlorinated hydrocarbons cannot be conducted in most industrialized countries because the discharge of these liquids into the environment is prohibited by law. Laboratory-validated numerical models provide a means to simulate such experiments without risk to the environment.

1.3 General Format for Model Construction

To construct a numerical model of a groundwater system, we first define, as closely as possible, the geological units and their hydrogeologic properties within the domain of interest. The domain should be selected such that conditions along its boundaries can be defined unambiguously.

If the model is designed for water quality studies, we then define processes that may play a role in the transport of contaminants. These processes will include, for example:

- groundwater flow,
- advective transport,
- dispersive/diffusive transport,
- chemical interactions,
- radioactive or biological decay,
- gravity forces,
- thermal processes,
- capillarity.

In most cases, only a limited number of these processes act at the same time. When the relevant processes are simple and act sequentially we speak of a linear system. For example,

advective-dispersive transport of a non-reacting dilute solute is a linear process. When the processes are coupled in complex relationships, or when the parameters controlling a process depend on the process itself, we speak of a nonlinear system. A nonlinear process occurs, for example, when the transport of a solute affects the flow system through the fluid density, or when an oxidation reaction depends on the amount of oxygen available while the oxygen available in turn depends on the amount consumed. Nonlinear systems are more difficult and costly to solve. While exact solutions are available for most linear problems, nonlinear problems are nearly always solved by means of numerical methods.

The processes taking place in a groundwater system are subject to physical laws such as:

- constitutive laws (Darcy's Law, Fick's Law),
- conservation laws for fluid mass, solute mass, thermal energy,
- force equilibrium laws.

These physical laws can be expressed mathematically in terms of governing equations which are usually partial differential equations. In cases of linear processes with simple geometry, these equations can generally be solved by analytical methods. In general cases involving nonlinear processes or complex geometry, the equations are solved numerically.

The mathematical description of the relevant physical laws, together with the description of the hydrogeology and the definition of the boundaries, constitute the *conceptual model* of the system. In order to solve the mathematical equations numerically, the system is *discretized* and the partial differential equations are approximated by algebraic equations at a finite number of points (*nodes*) in the domain. The *numerical solution* then solves the resulting sets of algebraic equations. Typically, several thousands of simultaneous equations are solved repeatedly in contaminant transport problems.

The entire solution process is formally expressed in a *computer code*. Although often the

computer code is seen as "the numerical model", the most important component is actually the conceptual model which has been selected to represent the real physical system and the processes taking place within this system. Thus great care must be taken in defining the conceptual model.

Model Verification, Validation and Calibration

Before the model can be applied to a real system, it must first be *verified* to ensure that the algebraic equations are solved correctly and that the code is error-free. This is generally done by comparison of model results with corresponding results produced by an analytical solution applied to a geometrically simple system subject to the same processes.

The model must also be *validated* (Tsang, 1991) to ensure that it actually represents the physical processes it is supposed to represent. This is done by comparing model results to field or laboratory observations. The comparison need not necessarily yield an exact agreement, but should provide proof that the physical/chemical/biochemical processes are validly and unambiguously represented in the model.

Disagreements between model results and field observation may be due to factors such as a lack of completeness in the data, measurement error, or less-than-perfect knowledge of the physical parameters. To obtain an improved match, the model can be *calibrated* by adjusting some of its parameters. However, only a small number of parameters can be adjusted in this way to preserve the *uniqueness* of the results. If different combinations of parameters values lead to the same result, the simulations will be non-unique.

Once the model is properly verified and validated, it can be applied to simulate the processes occurring in a real system, to perform sensitivity analysis, and to investigate "worst-case" situations. At this stage, the goal of the modeller should be to use the model to obtain the best possible insight into the system, and to use this insight in developing appropriate

strategies for achieving the overall objectives of the study.

1.4 Overview of Numerical Methods for Groundwater Models

The types of numerical methods that are most often used in groundwater modelling are *Finite Differences*, *Finite Elements*, and *Particle Tracking*. The first two of these approaches share the basic formulation of the solution as a boundary value problem. They originate from the two classical concepts of differentiation and integration in mathematics. The finite difference method has the advantage of being conceptually simple, while the finite element method is more flexible in representing domains with irregular geometry or anisotropic and heterogeneous media. In terms of accuracy, both methods are equivalent. Either of these two methods can be applied to the solution of flow and transport problems, and either allows the incorporation of chemical/biochemical interactions.

The user of numerical models should be aware of certain pitfalls which may affect the quality of the results obtained. One of these pitfalls is *numerical dispersion*, which may arise in the solution of the transport equation by either finite differences or finite elements. Techniques for its control have been developed and are easy to implement. Other pitfalls occur in the solution of nonlinear equations which describe flow in variably saturated porous media and transport with chemical or biochemical reactions.

The third of the commonly-used numerical methods, *Particle Tracking*, is applicable to the solution of transport problems only. This technique does not solve a boundary value problem, but instead considers the fate of contaminant particles as they migrate through the flow system. Particle tracking models are usually coupled with either finite difference or finite element models for determining the flow field. The main advantages of this technique are a simple and understandable concept, and a lack of susceptibility to numerical dispersion. A disadvantage is that chemical/biochemical interactions cannot be easily incorporated in a general way. The method is particularly useful for the simulation of hydraulic remediation

measures.

An excellent text on groundwater modelling at the introductory level is Kinzelbach (1986). Huyakorn and Pinder (1983) give an advanced treatment of numerical methods with a strong mathematical basis. Luckner and Schestakow (1986) present a comprehensive survey of all types of migration processes in groundwater, with some basic numerical methods. Other texts of valuable topics include Wang and Anderson (1982), Bear and Verruijt (1987); and Molson *et al.* (in preparation).

2. REVIEW OF GOVERNING EQUATIONS

The main equations that govern the physics of groundwater flow and contaminant transport are the Darcy equation, the groundwater flow equation, and the transport equation. These are supplemented by the appropriate relationships expressing chemical and biochemical transformations.

2.1 Darcy Equation

The Darcy equation relates the flow of water through a porous medium to the driving force, which is the hydraulic gradient. In general, natural groundwater systems are anisotropic (i.e. exhibiting preferred directions of flow) due to geologic factors such as the sedimentary structure of the medium, or fracturing. In the case of anisotropy due to the sedimentary structure, flow parallel to the layering is generally favoured over flow across the layering.

The general form of the Darcy equation for three dimensional (3D) anisotropic media is (Bear, 1979; Freeze and Cherry, 1979):