

# Part I

## **The Essentials of Dissolved Species Transport in the Subsurface Environment: Basic Definitions, Fundamental Mechanisms and Mathematical Formulation**

The theory of solute migration in groundwater originates from studies devoted to the description of elementary pore-scale mechanisms (processes) of the movement of dissolved species in a single fluid phase, including advection, molecular diffusion, and hydrodynamic dispersion, which are accompanied by acts of simplest sorption-type physicochemical interactions and solute decay (destruction) reactions. Those studies were mostly based on the classical theory of fluid motion in idealized porous media (Muskat 1937; Scheidegger 1957), as well as on chemical kinetics and reaction engineering. However, it has become clear that there exist some specific features in the application of conventional hydrodynamics methods to the formulation, solution, and analysis of many practically significant hydrogeological problems. In particular, the relative significance of those mechanisms and interactions in the general migration process was soon found to depend on the spatial and temporal scale of their analysis, the lithological and genetic type of geological sections, and the spatial correlation structure of their physical parameters, the structure of water flows, and the conditions on their inner and outer boundaries. This, as well as the specific features of the application of physico-mathematical apparatus to the solution of appropriate boundary problems regarding dissolved species transport in single-phase constant-density groundwater flows, will be the focus of the first part of this book.

Mathematical models used to describe solute transport in the unsaturated zone of the subsurface are also included in this part of the book. As will be shown, for accurate prediction of contaminant transport through the unsaturated zone, field equations for transport of moisture and chemicals must be coupled.

The equations given here represent a deterministic approach to describing the subsurface transport phenomena, and have been assembled from a considerable collection of previous works and investigations conducted by many recognized

authorities in the field of subsurface fluid dynamics. More generalized fluid flow and transport models, accounting for the stochastic nature of aquifers and soil materials are subject of high profile, well-publicized special investigations.

The proposed material forms a bridge to the understanding of solute transport under near-natural conditions and the analysis of migration of complex-composition solutions (liquids) whose properties differ from those of formation waters. Besides, the approaches developed here will be used to assess the contributions of various physicochemical processes, which in many cases control the potential of anthropogenic impact on groundwater quality under natural conditions.