Chapter 1
Introduction

The unsaturated zone, also called vadose zone, is located between the soil surface and the groundwater table. Its depth is variable and depends on geological and climatic factors. As the name implies, soils and rocks in the unsaturated zone are only partially filled with water, the rest of the pore space being occupied by air. The vadose region constitutes a vital link between groundwater, atmospheric water and surface water. It is a place of intense human activity of various kinds, including civil and environmental engineering and agriculture. Therefore, flow and transport phenomena occurring in the unsaturated zone can be studied from different viewpoints, as shown schematically in Fig. 1.1.

A distinct scientific specialization, soil physics, is entirely devoted to the study of physical processes in soils, including the water flow in unsaturated conditions, e.g. [17, 20, 47]. Soil physics developed in a close relationship to agronomy and hydrology. In agricultural applications, emphasis is put on the availability of water and dissolved nutrition substances to plants, which motivates the development of comprehensive models to describe the soil-plant-atmosphere system, e.g. [8, 9]. Accurate evaluation of water infiltration into the soil and evapotranspiration from the soil is also important for hydrological models. For instance, the infiltration capacity of soils has a direct influence on the formation of runoff, and thus is an important factor in predicting the risk of flood. Consequently, a trend towards explicit coupling of the surface and shallow subsurface flow in hydrological models can be observed, e.g. [11, 48].

On the other hand, the water flow processes in the unsaturated zone have significant impact on groundwater flow in saturated aquifers, which constitute a major source of drinking water. Even more importantly, the vadose zone is a buffer between groundwater and various sources of pollutants located at the soil surface or in the shallow subsurface. Reliable prediction of the fate of contaminants dissolved in water requires the knowledge of water flow velocities in the unsaturated zone, which are in general highly variable in space and time. Therefore, increasing attention is paid to coupled saturated-unsaturated models of groundwater flow and contaminant transport, e.g. [43, 44, 50]. Moreover, accounting for the unsaturated flow allows for

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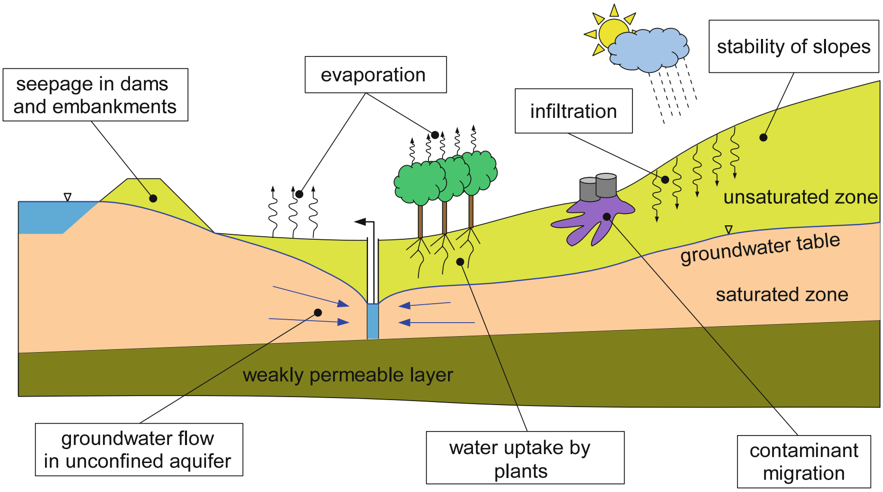

Fig. 1.1 Typical problems related to water flow in the vadose zone

improved estimation of parameters related to the hydraulics of phreatic aquifers, such as the recharge rate [18], the specific yield [35] or the height of the seepage face in wells [5].

Water flow in the vadose zone has important implications also for geotechnical engineering. Traditionally, soil mechanics focused mostly on completely dry or fully saturated non-cohesive soils, and fully saturated cohesive soils. However, a wide range of problems can be more accurately modelled, if the variability in the soil water saturation is taken into account. This is particularly necessary for soils that swell, shrink or collapse due to the changes in water saturation, but there is an increasing awareness of the importance of unsaturated flow also for other applications, including soil compaction, slope stability, flow in dams and embankments, protection of landfills, tunneling or interpretation of penetration tests, e.g. [30, 31, 51]. Unsaturated soil mechanics is still an emerging and very active field of research, which developed substantially during the last twenty years, e.g. [10, 25, 28].

In all the applications mentioned above a crucial issue is the ability to accurately model water flow in soils, or—more generally—partially saturated porous media. This, however, is a challenging task, due to the multi-phase and multi-scale nature of porous media, especially the ones formed by natural processes. Porous soils and rocks in the vadose zone consist of several deformable solid and fluid phases, separated by clearly distinguishable interfaces, representing sharp discontinuities in physical and chemical properties [16, 33]. In general, each of the phases consists of multiple chemical components, which can move between phases. Pore air, for instance, is a mixture of gases, including water vapor, while pore water contains many dissolved substances, including gases. The number of phases and components included in the mathematical model depends on the problem under consideration. In many applications focusing on the water flow, a sufficient accuracy can be achieved with

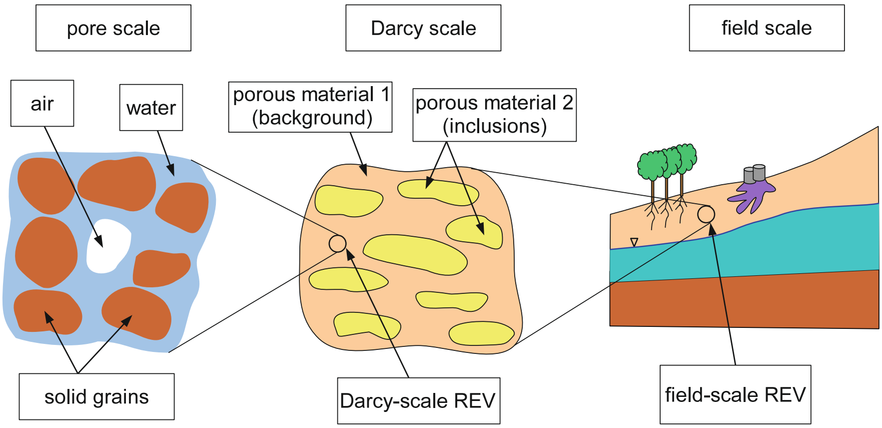

Fig. 1.2 Observation scales in a porous medium

a simplified model, where both air and water are considered as immiscible single-component phases and the deformation of the solid skeleton is neglected. Such an approach is adopted in the present work.

Modelling of flow in porous media is further complicated by the fact that the relevant physical processes can be described at various observation scales. Mathematical models applied at each scale typically represent the principles of conservation of basic quantities such as mass, momentum and energy, but the exact form of the governing equations may differ substantially between the scales. In some cases the model describing processes at a larger scale can be derived directly from the equations relevant at a smaller scale by an appropriate averaging procedure. This process is known as upscaling. Alternatively, the governing equations can be formulated directly at the larger scale, based on phenomenological considerations. Two basic scales, typically distinguished in porous media, are the pore scale and the Darcy scale, Fig. 1.2. In the former case, the characteristic spatial dimension is the size of a single pore, which in granular media is approximately proportional to the grain size. At this scale, each phase occupies a distinct spatial domain, and each point of space can be associated with a specific phase. On the other hand, it is assumed that each phase can be regarded as a continuum within its own spatial sub-domain, i.e. the size of the pores is much larger than the size of fluid molecules. The flow of fluid phases can be described by the Navier-Stokes equations with appropriate conditions at the fluid-solid and fluid-fluid interfaces. However, the pore scale description is not suitable for practical problems, which involve spatial domains having dimensions larger than the pore size by many orders of magnitude. Therefore, the governing equations describing behaviour of various phases are usually formulated at a much larger scale, which in the present work will be referred to as the Darcy scale, from the name of H. Darcy, who developed the well-known formula for the water seepage velocity in a porous medium [7]. At this scale, each spatial point corresponds to a representative elementary volume (REV), containing a sufficiently large number of pores, occupied by multiple fluid phases. Thus, in contrast to the pore scale description, at the Darcy scale each phase forms a continuum over the entire spatial domain.

The most commonly used two-phase model of air and water flow at the Darcy scale is a combination of the mass conservation equation for each fluid with the semi-empirical equation for flow velocity, based on an extension of the Darcy formula for the case of multi-phase flow. One of key components of the model is the capillary function, describing the relationship between the water saturation and the capillary pressure, defined as the difference between pressures in the air and water phases. A complementary constitutive relationship is given by the relative permeability function, which describes the ability of each fluid phase to flow in the porous medium as a function of the phase saturation. Both functions are strongly nonlinear. Their form depends principally on the geometrical characteristic of the pore space and on the properties of the fluid-fluid and fluid-solid interfaces (surface tension). The mathematical model of two-phase flow is often formulated as two coupled partial differential equations of parabolic type, with the two phase pressures or saturations as the primary unknown variables.

The two-phase model can be simplified, if one assumes that the air phase is continuously distributed in pores, it is connected to the atmospheric air and much more mobile than the water phase. Accordingly, the pressure in the air phase can be considered constant and equal to the atmospheric pressure, and the equation describing air flow is eliminated. The remaining equation for the water flow is called the unsaturated flow equation or the Richards equation [34]. Similarly to the full two-phase flow model, the Richards equation is based on semi-empirical concepts of the capillary and relative permeability functions, introduced at the Darcy scale to account for a number of pore scale phenomena, which at present are not fully understood. These constitutive relationships are difficult to associate with the Darcy-scale processes in a manner that is both physically rigorous and easy to implement practically. While a number of improved formulations for the two-phase and unsaturated flow have been proposed, e.g. [3, 14, 26, 29, 32, 49], the Richards equation remains a useful and well-established tool in the unsaturated zone modelling, and is the basis of the present analysis.

The present book focuses on two aspects of the application of the Richards equation. The first one is related to its numerical solution. Although significant development of the numerical algorithms occurred in the last twenty years, e.g. [4, 27], solution of the Richards equation remains a challenging task due to the afore-mentioned strongly nonlinear constitutive relationships, which must be appropriately represented in the discretized space-time domain. A particularly important issue is the approximation of the relative permeability between the nodes of a spatial grid, which is a necessary to estimate water fluxes, according to a discrete version of the Darcy formula. As the relative permeabilities may differ by several orders of magnitude (for example, during infiltration in a dry soil, or evaporation), the choice of the averaging method is often essential for the overall accuracy of the approximate solution. Several simple averaging schemes have been proposed, e.g. arithmetic mean, geometric mean and upstream weighting, but each of them may lead to large errors for particular combinations of the initial and boundary conditions, grid size and the form of functional relationship between the relative permeability and the capillary pressure, e.g. [1, 2, 15]. On the other hand, more accurate methods often require significantly larger computational effort, e.g. [46]. In this work an averaging scheme is presented, that is relatively easy to implement and significantly improves the solution accuracy for a wide range of one- and two-dimensional problems. The method was proposed in the paper [36], and further developed in [37, 38]. Extension of the method for unstructured grids and implications for the solution of the full two-phase model are also discussed. The analysis is carried out for a simple form of the Richards equation, which does not account for soil compressibility nor water uptake by plant roots. While these two factors are very important in many applications related to the unsaturated zone and must be properly treated numerically, they have no direct influence on the development of the averaging schemes for inter-nodal permeabilities.

The second topic considered in this book deals with flow in porous media showing material heterogeneity at the Darcy scale. Heterogeneity may be related to various physical and chemical properties of the porous medium. The focus of this work is on porous formations composed of sub-domains characterized by distinct textural properties, which imply differences in pore geometry, and consequently in the physical parameters such as permeability, hydraulic diffusivity or air entry pressure (defined as the value of the capillary pressure above which the pore air flow is possible). The important issue of chemical heterogeneity, for instance related to the wettability and adsorption properties of the solid phase is not considered here. If the number of heterogeneous regions in the considered spatial domain is large, their explicit representation on a numerical grid becomes difficult or even impossible. Therefore, a new observation scale can be introduced, which for the purposes of this work will be called the field scale, Fig. 1.2. At this scale the relevant representative elementary volume encompasses sufficiently large number of Darcy scale heterogeneities to allow for the development of an upscaled model. The heterogeneous structure can be described in either deterministic or stochastic terms. In particular the stochastic models for flow and transport in unsaturated heterogeneous porous media have been a subject of intense research, e.g. [6, 12, 52]. In this book the deterministic viewpoint is adopted and a specific heterogeneity pattern is considered: a binary porous medium with disconnected porous inclusions (lenses) embedded in a continuous porous background material. While such a structure is relatively simple, it is representative of a number of natural porous formations, such as fluvial or coastal sediments, or sandstone-shale sequences, e.g. [19]. On the other hand, this type of pattern can be conveniently parametrized and analysed from the theoretical point of view, allowing for a good general understanding of local heterogeneities on the large-scale behaviour of the medium. The second part of this work presents an extended discussion of several models based on the Richards equation, which were developed for such type of media using the asymptotic homogenization approach [21–24, 39, 41]. These works showed that the macroscopic behaviour of the medium depends on the ratio between the permeabilities of the inclusions and the background material. A generalized model, valid for a wide range of inclusion-to-background permeability ratio, was proposed [39], and its preliminary experimental verification was carried out [40]. It can be also shown that the Richards approximation is not valid for media characterized by higher value of the air-entry pressure in the matrix than in inclusions. In porous media showing heterogeneity with respect to the air-entry pressure the assumption of the continuity of air phase in porous medium, which underlies the Richards equation, may not be satisfied [41]. However, the accuracy of the Richards equation can be improved, if the large-scale capillary and permeability functions are appropriately modified [42].

The field scale discussed in this book represents an intermediate level in the hierarchy of scales relevant to the modeling of water flow in the vadose zone, with the characteristic length of the order of meters to dekameters. Significant research has been devoted to the description of unsaturated zone processes at regional scale, corresponding to hydrological watersheds, with the horizontal dimensions of many kilometers, e.g. [13, 45]. At such a scale, simplified mathematical models of the black-box type are routinely used and an important question is how to relate their parameters to the more detailed characteristics of the porous media available at smaller scales. While regional-scale hydrological modelling is of high practical importance, it is not considered in this book.

The book is structured as follows. Chapter 2 presents the mathematical formulation of flow in unsaturated porous medium. The governing equations for the two-phase model and the Richards model are discussed, together with various analytical formulae for capillary and permeability functions. In Chap. 3 a numerical algorithm to solve the governing flow equations is developed. The algorithm is formulated in general terms and can be applied to both the two-phase model and the Richards equation. Various methods of spatial discretization are discussed, including the control volume–finite difference and control volume–finite element approaches. The approximation of the average permeability in spatially discretized Richards equation is considered in detail in Chap. 4. Chapter 5 introduces basic concepts of upscaling. In Chap. 6 the upscaled models developed for flow in binary media without air-entry pressure effects are presented. The model accounting for air-entry effects is discussed in Chap. 7. The final chapter summarizes the contents of the book and outlines some open problems related to the discussed topics.

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