Modeling of Unsaturated Water Flow in Highly Heterogeneous Soils

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JURY

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Grenoble, 26 October 2004
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Notation

Only significant symbols are listed.
Subscripts 1 and 2 refer to the highly conductive sub-domain and the weakly conductive sub-domain respectively.
Subscripts a and w refer to air and water respectively.

Acronyms

<table>
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<th>Description</th>
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<tr>
<td>BC</td>
<td>Brooks – Corey (1964) hydraulic functions model</td>
</tr>
<tr>
<td>DPH</td>
<td>double-porosity model obtained by homogenization</td>
</tr>
<tr>
<td>DPGG</td>
<td>double-porosity model of Gerke and van Genuchten (1993a)</td>
</tr>
<tr>
<td>FS</td>
<td>fine scale solution</td>
</tr>
<tr>
<td>SP</td>
<td>single porosity model</td>
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Latin letters

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<th>Symbol</th>
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<td>capillary capacity, [L^{-1}]</td>
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<td>C^<em>_1, C^</em>_2</td>
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<td>C^{eff}</td>
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<td>f_1, f_2</td>
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<td>g</td>
<td>gravitational acceleration, [L T^{-2}]</td>
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Greek letters

\( \alpha \) retention function parameter (VGM), [L\(^{-1}\)]
\( \beta \) geometry coefficient (DPGG), [-]
\( \gamma_w \) scaling coefficient (DPGG), [-]
\( \Gamma \) interface between \( \Omega_1 \) and \( \Omega_2 \)
\( \Delta X \) spatial interval in the solution of the macroscopic model, [L]
\( \Delta Y \) spatial interval in the solution of the local flow in inclusions, [L]
\( \Delta t \) time step, [T]
\( \varepsilon \) scale parameter, [-]
\( \zeta \) normalized surface-to-volume ratio for inclusions (DPGG), [-]
\( \eta \) conductivity function parameter (BC), [-]
\( \theta \) volumetric water content, [-]
\( \theta_r \) volumetric water content, [-]
\( \theta_s \) volumetric water content, [-]
\( \lambda \) retention function parameter (BC), [-]
\( \mu \) dynamic viscosity [M L\(^{-1}\) T\(^{-1}\)]
\( \nu \) direction coefficient in the one-dimensional flow equation, [-]
\( \xi \) weighting parameter in the time-discretization scheme, [-]
\( \rho \) volumetric density [M L\(^{-3}\)]
\( \rho_d \) bulk density [M L\(^{-3}\)]
\( \rho_s \) skeletal density [M L\(^{-3}\)]
\( \tau_{ABS} \) absolute error tolerance, [L]
\( \tau_{REL} \) relative error tolerance, [-]
\( \Phi \) objective function in the inverse analysis, [L\(^2\)]
\( \chi \) solution of the local boundary value problem, [-]
\( \Omega \) period
\( \Omega_1 \) highly conductive part of the period
\( \Omega_2 \) weakly conductive part of the period
Chapter 1

Introduction

1.1 Presentation of the problem

In recent years increasing attention is directed towards modeling of transport processes in the unsaturated zone. The unsaturated zone (or vadose zone) is positioned between the soil surface and the groundwater level, constituting key element in the hydrological cycle. Various chemical substances move with infiltrating water through the vadose zone and can contaminate the groundwater. The nature of the pollutants may be very different (fertilizers, pesticides, pathogenic microorganisms, radio-nuclides, non-aqueous liquids and others) and they can originate from different sources (agricultural and industrial activity, accidental spills, subsurface tanks, waste disposals). The prediction of the fate of pollutants is crucial for protection of the groundwater resources. Thus, accurate qualitative and quantitative description of water flow in the vadose zone is required. Other important domains concerned by the unsaturated flow problems include agriculture, forestry, large-scale modeling of hydrological systems or civil engineering (e.g. stability of slopes and earth dams).

Simulation of flow in the vadose zone is a complicated task for some reasons. One reason is the nonlinearity of the governing equations. At least two fluid phases (i.e. water and air) are present in the unsaturated soils. Although the full two-phase flow model can be replaced in many situations by a simplified unsaturated flow equation (Richards, 1931), the constitutive relations used in the latter model are still of highly nonlinear character. Another important problem is the heterogeneity of the modelled systems. Like all the geological porous media soils and rocks in the unsaturated zone exhibit heterogeneities at various observation scales. Usually, the scale of local heterogeneities is much smaller than the scale of the considered transport process. Also, a detailed information about the local structure of the medium is hardly accessible. Thus, from the practical point of view, the explicit representation of the heterogeneity is impossible. It is necessary to develop mathematical models that treat the
medium as homogeneous and describe it by some average parameters. On the other hand such equivalent models should properly take into account the influence of heterogeneities at different scales.

A large class of heterogeneous porous formations can be described as double-porosity media. They are composed of two sub-domains characterized by contrasting hydraulic properties. Typical examples are aggregated soils or fractured rocks. In such media one can distinguish three different observation scales (see Fig. 1.1). In this study the microscopic scale is associated with grains and pores. The local scale (also known as mesoscopic or Darcy scale corresponds to the characteristic dimension of heterogeneities (e.g. aggregate diameter or fracture spacing). Finally, the macroscopic scale represents the domain of practical interest which contains large number of heterogeneities.

The heterogeneous structure of double-porosity media may result from different physical, chemical and biological processes, which are the origin of fractures, fissures, vugs, shales, aggregates, macropores or cracks. Consequently, the double-porosity media can further be divided into several classes. One class of double-porosity structure is represented by media with the two porous sub-domains occupying similar fraction of space, where the water flow in both regions can be described by the Richards equation. For example, one can think about aggregated soils, with distinct inter-aggregate region filled by coarser material, sand formations with clay lenses or sandstone with sand shales. This type of media is widespread in nature and it is the subject of the present study. Other types of dual-porosity structures are fractured rocks or soils with large fissures or macropores, which appear due to the shrinkage, growth of plants (root channels) or biological activity (wormholes). There is also a group of porous media containing separated fissures, large pores (vugs) or cavities which are not connected with each other. In all those cases the highly conductive structures have often over-capillary size. Thus, the Richards equation may be inadequate to describe water flow in such media and other mathematical formulations are proposed.

Due to their particular structure double-porosity media often show non-standard behavior at the macroscopic scale. The characteristic time of flow is very different in each region. The time required to equilibrate pressure and saturation is much longer in the weakly conductive aggregates than in the highly conductive system. It means that non-equilibrium conditions may appear during flow and transport processes. If the highly conductive regions are interconnected they will transmit most of the water, while the less conductive regions are bypassed. This phenomenon is described as preferential flow or bypass flow (Jarvis, 1998). The influence of heterogeneous soil structure on the water propagation has been reported by many authors (Smettem et al., 1991; Larsson et al., 1999; Ludwig et al., 1999; Kätterer et al., 2001; Šimůnek et al., 2001; Gerke & Köhne, 2004, among many others). While the
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**microscopic scale**
- pores
  \[ l' \approx 10^{-6} \text{ m} \div 10^{-3} \text{ m} \]

**local (mesoscopic) scale**
- soil heterogeneities
  \[ l \approx 10^{-2} \text{ m} \div 10^{-1} \text{ m} \]

**macroscopic scale**
- practical problems
  \[ L \approx 10^{1} \text{ m} \div 10^{3} \text{ m} \]

**Figure 1.1:** Observation scales and characteristic lengths in a double-porosity medium.
preferential flow refers to the acceleration of flow with regard to the weakly conductive soil matrix, one can assume different point of view and consider the presence of aggregates as the retardation factor which slows down the flow in the more conductive domain. It leads to the so-called tailing effect, which may be important during the remediation of polluted soils, for example. None of those effects can be described using classical Richards equation with averaged parameters.

In the last decades many models for non-equilibrium flow and transport in double-porosity media have been proposed. The two-equation phenomenological models based on some empirical considerations, initially introduced by Barenblatt et al. (1960), are widely used in hydrology, groundwater and petroleum engineering (Bear et al., 1993; Chen, 1989; Šimůnek et al., 2003). The double-porosity medium is conceptualized as two continuous overlapping sub-domains. The flow in each region is described by separate equation. The equations are coupled by a source term representing water transfer between sub-domains. The transfer rate is related to the difference of the pressure heads or the saturations in the two regions.

Alternatively the macroscopic models can be obtained using mathematically rigorous up-scaling methods. In this approach the model is derived from the description of physical process at local scale. The corresponding macroscopic equations can be obtained by different methods, for example the volume averaging method (Quintard & Whitaker, 1987; Whitaker, 1999) and the asymptotic homogenization method (Bensoussan et al., 1978; Sanchez-Palencia, 1980; Auriault, 1991). Such approach has considerable advantages. In the homogenization method no assumptions are made on the form of the macroscopic model and the derivation is mathematically rigorous. Although the up-scaling methods have been extensively used to study flow in dual-porosity media, relatively few papers addressed specifically the problem of flow in unsaturated zone (Hornung, 1991; Lewandowska & Laurent, 2001).

1.2 Objective and scope of the study

This study is aimed at the analysis of flow in the unsaturated double-porosity soils using the homogenization method. The work has three main objectives. First is the development of the macroscopic flow models starting with the description at the local (Darcy) scale. The second objective is the numerical implementation of the mathematical models. The third aim is to compare the results obtained by homogenization with other existing approaches and with the experimental results.

The structure of this work follows the outlined objectives. In Chapter 2 an overview of the existing models is presented. First, the mathematical formulation of flow at the local scale is recalled, including the full two-phase model and the Richards equation. In the second part
we present various models of flow in heterogeneous soils. We focus on the non-equilibrium models, particularly the double-porosity approach, which is widely used in hydrology and petroleum engineering. Phenomenological formulations as well as the results obtained using mathematically rigorous up-scaling procedures are discussed. Finally, some numerical and experimental issues related to the flow in double-porosity soils are presented.

Chapter 3 contains the major theoretical part of the work, which is the derivation of the macroscopic models for flow in double-porosity soils by the asymptotic homogenization method. The starting point is the description of flow at the local scale. We assume that locally the flow is governed by the Richards equation. Two distinct soil structures are examined: soil with the highly conductive regions interconnected and soil with highly conductive inclusions embedded in a less conductive matrix and separated from each other. The hydraulic parameters of the two components are very different. For each structure we provide the macroscopic model and the definition of effective parameters. The results are compared with the model obtained for moderately heterogeneous soils (Lewandowska & Laurent, 2001) and other models existing in literature.

Numerical implementation of the models is presented in Chapter 4. The application includes two main elements: calculation of the effective parameters and solution of the macroscopic flow problem. In case of the non-equilibrium flow, the macroscopic model has the form of highly nonlinear integro-differential equation. It requires special numerical approach. A program DPOR-1D has been developed, which simulates macroscopically one-dimensional flow in soils with three-dimensional local structure. The algorithm is based on the fully implicit finite difference formulation combined with Newton nonlinear solver. More details about the DPOR-1D code are provided in the appendices.

In Chapter 5 we present the calculation of the effective conductivity for double-porosity media. The calculations are performed for two types of media, i.e. soils with inclusions highly conductive or weakly conductive with respect to the matrix. Several factors influencing the effective conductivity are examined: the geometric form of inclusions, their volume fraction and their spatial arrangement. The values obtained from homogenization are compared to the theoretical bounds for effective conductivity existing in the literature.

Numerical solutions of some macroscopic flow problems in double-porosity soils are presented in Chapter 6. Three different soil structures are examined. We consider macroscopically one-dimensional infiltration in an initially dry soil. The numerical simulations performed by DPOR-1D code based on the homogenization approach are compared with the simulations using phenomenological dual-porosity model of Gerke & van Genuchten (1993a) and with the fine scale solution where the heterogenous structure of the medium is explicitly represented. The latter solution is treated as the reference one, since we assume that it
represents exactly the behavior of the heterogeneous soil.

Chapter 7 describes the experimental verification of the non-equilibrium flow model. The experiments were carried out on a double-porosity medium consisting of a mixture of sand and sintered clayey spheres arranged periodically. A series of infiltration tests were performed on a 60 cm high column filled with air-dry medium. Additional experiments were carried out on pure sand and clayey material in order to obtain the hydraulic characteristics of both materials. The experimental results are compared with the numerical simulation by DPOR-1D code.

Finally, the obtained results are summarized in Chapter 8. This chapter presents major conclusions coming out of the study. Moreover, some perspectives of future research are outlined.
Chapter 2

State of the art

2.1 Introduction

This chapter presents an overview of the literature on the flow in double-porosity soils. We focused on some key issues, which are related to the further part of this work. First, the mathematical models of two-phase and unsaturated flow at the local scale are presented (Section 2.2). Then, we discuss the macroscopic models (Section 2.3), which are obtained using either phenomenological approach or up-scaling methods. The models can be divided into three groups, which correspond to different types of soils: (i) moderately heterogeneous, (ii) highly heterogeneous with the more conductive regions interconnected and (iii) highly heterogeneous with the more conductive regions disconnected. In Section 2.4 some problems concerning the numerical implementation of the models are outlined. Finally, the experiments related to the flow in double-porosity soils are presented in Section 2.5.

2.2 Description of flow at the local scale

In this study we are interested in the development of macroscopic scale models of flow in double-porosity soils. The starting point for our analysis is the description of flow at the local (Darcy) scale. Under this term we understand the scale much larger than the scale of single pores, where continuum description of the porous medium may be introduced and where the soil is supposed to be homogeneous, so that the Darcy’s law is valid. The physical variables appearing in the governing equations represent values averaged over some representative elementary volume (REV), which incorporates large number of grains and pores (Bear, 1972), but is very small compared to the characteristic size of the considered porous region. The governing equations for flow in porous media presented in the following sections are discussed in more detail in the works of Scheidegger (1957), Bear (1972), Chavent
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2.2.1 The two-phase flow model

The soil in the unsaturated zone can be considered as a three-phase medium. It consists of solid grains with the pore space occupied by air and water (see Fig. 2.1). In this study we assume that the soil is rigid, the flow is isothermal and the two fluid phases are immiscible. We neglect the vapor flow, the interphase phenomena and the presence of dissolved substances in water. Under these hypotheses the mass balance for each fluid phase is represented by the following equations (Bear, 1972; Chavent & Jaffre, 1986):

\[ m \frac{\partial (\rho_a S_a)}{\partial t} + \nabla \cdot (\rho_a q_a) = 0 \]  \hspace{1cm} (2.1)

\[ m \frac{\partial (\rho_w S_w)}{\partial t} + \nabla \cdot (\rho_w q_w) = 0 \]  \hspace{1cm} (2.2)

where the subscripts \( a \) and \( w \) refer to the air and water phase respectively, \( m \) is the medium porosity, \( \rho_i \) is the fluid density, \( S_i \) is the saturation of the given fluid phase, \( q_i \) is the volumetric fluid flux and \( t \) is time. The fluxes \( q_a \) and \( q_w \) are given by the generalized Darcy’s law, which relates the flux to the potential gradient (Darcy, 1856; Buckingham, 1907; Muskat et al., 1937):

\[ q_a = -K_{ra}(S_a) \frac{k}{\mu_a} \nabla (p_a + \rho_a g X_3) \]  \hspace{1cm} (2.3)

\[ q_w = -K_{rw}(S_w) \frac{k}{\mu_w} \nabla (p_w + \rho_w g X_3) \]  \hspace{1cm} (2.4)

where \( k \) is the absolute permeability tensor, \( K_{ri} \) is the relative permeability of given fluid phase, \( \mu_i \) is the dynamic viscosity coefficient of the given fluid phase, \( p_i \) is the fluid pressure, \( g \) is the gravitational acceleration and \( X_3 \) is the vertical spatial variable (oriented positively upwards). The relative permeability depends on the saturation of each phase. The Darcy’s law represents the conservation of momentum for the flow in porous media when the inertial effect can be neglected. The passage from the pore-scale Navier-Stokes equations to the Darcy’s law was shown for example by Bear (1972) and Whitaker (1986) for saturated flow and by Auriault (1987) for unsaturated flow.

The pore space is completely filled by two fluids, which implies the following relation:

\[ S_a + S_w = 1 \]  \hspace{1cm} (2.5)

The fluids are separated by a curved interface, which contacts the solid phase surface at a specific angle, known as the wetting angle. In our case water is the wetting fluid, whereas air
Figure 2.1: Microscopic view of soil in the unsaturated zone.

is the non-wetting fluid. Due to the existence of the interfacial tension the pressure in the non-wetting fluid is higher than in the wetting one. The difference is known as the capillary pressure:

\[ p_a - p_w = p_c(S_w) \]  \hspace{1cm} (2.6)

The value of the capillary pressure depends on the volumetric content of the two fluid phases. Usually it is expressed as a function of the wetting fluid saturation \( p_c = p_c(S_w) \) (Leverett, 1941; Chavent & Jaffre, 1986).

The equations (2.1)–(2.6) form a complete mathematical model of two-phase capillary flow at the local scale. The solution of this system requires the knowledge of the constitutive relations for \( K_{rw}(S_w) \), \( K_{ra}(S_w) \) and \( p_c(S_w) \).

2.2.2 The Richards model

When the general two-phase flow model is applied to the flow in the unsaturated zone of soil one often assumes that the air pressure is constant and equal to the atmospheric pressure (Richards, 1931; Hillel, 1980; Kutilek & Nielsen, 1994). In other words the mobility of air is much greater than the mobility of water. This hypothesis seems to be justified in many practical situations, although the question about its validity persists (Gray & Hassanizadeh, 1991a,b; Vachaud et al., 1973; Touma & Vauclin, 1986; Tegnander, 2001). Assuming additionally that water compressibility in the unsaturated zone can be neglected, one obtains a simplified description of water flow in soils.

The governing equation is written using physical variables slightly different than the ones appearing in (2.1)–(2.6). The volumetric water content \( \theta \) is commonly used instead of water
saturation:
\[ \theta = m S_w \quad (2.7) \]

Since the air pressure is assumed to be constant, the water potential is expressed in terms of the water pressure head:
\[ h = \frac{p_c}{\rho g} \quad (2.8) \]

The variable \( h \) is also known as capillary pressure head, matrix head or suction potential. It defines the potential of soil water related to the atmospheric pressure. The water pressure head assumes negative values in the unsaturated conditions and positive values in the saturated conditions. It should be noted that the potential of soil water in the unsaturated region is related not only to the capillary forces, but also to adsorptive forces, which become predominant in very dry conditions (Kutilek & Nielsen, 1994). Since the density and viscosity are assumed constant, the water transfer properties can be characterized by the hydraulic conductivity tensor \( K \):
\[ K = k \frac{\rho g}{\mu} \quad (2.9) \]

Using those variables one can recast (2.2) into the well-known Richards equation (Richards, 1931; Bear, 1972; Kutilek & Nielsen, 1994):
\[ \frac{\partial \theta}{\partial t} - \nabla \cdot (K \nabla (h + X_3)) = 0 \quad (2.10) \]

Due to the relation between saturation and capillary pressure head \( h \) the equation (2.10) can be rewritten as:
\[ C \frac{\partial h}{\partial t} - \nabla \cdot (K \nabla (h + X_3)) = 0 \quad (2.11) \]
where \( C \) is the capillary capacity or specific water capacity. It is defined as:
\[ C(h) = \frac{d\theta}{dh} \quad (2.12) \]

It is also possible to rewrite (2.10) in terms of the volumetric water content:
\[ \frac{\partial \theta}{\partial t} - \nabla \cdot (D \nabla \theta + K \nabla X_3) = 0 \quad (2.13) \]
where \( D \) is the capillary diffusivity or hydraulic diffusivity:
\[ D(h) = \frac{K(h)}{C(h)} \quad (2.14) \]

The equations (2.10), (2.11) and (2.13) are known as mixed, pressure-based and moisture-based form of the Richards equation, respectively.
2.2.3 Hydraulic functions

The solution of equation (2.10) or (2.11) requires the knowledge of hydraulic properties of the soil given by the retention function (i.e. the $\theta - h$ relation) and the conductivity function ($K - h$ or $K - \theta$ relation). Both functions are highly nonlinear. For practical purposes the hydraulic functions are defined by some closed-form analytical expressions. Such expressions were proposed by numerous authors, including Mualem (1976), van Genuchten (1980), Burdine (1953), Gardner (1958), Brutsaert (1966), Brooks & Corey (1964), Kosugi (1994), Rossi & Nimmo (1994), Bumb et al. (1992), Laliberte (1969), Childs & Collis-George (1950) among many others — see for example (Leij et al., 1997) or (Kosugi et al., 2002) for a more detailed presentation and comparison of different propositions.

Fig. 2.2a presents typical retention curves for three different soil textural classes (parameters taken from Carsel & Parrish (1988)). The maximum value of water content is the saturated water content $\theta_s$, which by definition corresponds to $h = 0$. For decreasing $h$ the water content tends to a limit minimum value $\theta_r$, known as the residual water content. Thus, the water content varies in the range $(\theta_r, \theta_s)$ and it is convenient to define the effective saturation:

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r}$$  \hspace{1cm} (2.15)

For many soils $\theta$ remains nearly constant for $h$ lower than 0 and starts to decrease at some value $h_a$, which is defined as the air-entry pressure head. Usually the $\theta - h$ curve shows an inflection point $h_{inf}$. The form of the retention curve is related to the pore-size distribution of the soil.

Brooks & Corey (1964) introduced following expression for the retention function:

$$S_e = \left(\frac{h_a}{h}\right)^\lambda \quad h < h_a$$

$$S_e = 1 \quad h \geq h_a$$  \hspace{1cm} (2.16)

where $\lambda$ is an empirical parameter characterizing pore-size distribution. This model does not include inflection point, but defines a distinct air-entry pressure. Note that the capillary capacity is discontinuous at $h_a$.

Another commonly used model was proposed by van Genuchten (1980):

$$S_e = [1 + (\alpha|h|)^n]^{-m}$$  \hspace{1cm} (2.17)

where $\alpha$ is a scaling parameter related (but not exactly corresponding) to the inverse of the inflection point pressure $h_{inf}$. The dimensionless parameters $m$ and $n$ may be fitted independently, although usually it is assumed that $m = 1 - 1/n$ (Mualem’s condition, (Mualem, 1976)) or $m = 1 - 2/n$ (Burdine’s condition, (Burdine, 1953)).
Figure 2.2: Typical retention functions (a) and typical conductivity functions (b) for three soil textural classes.

Similarly to the retention function, the conductivity function is highly nonlinear. It can be presented as:

\[ K = K_r K_s \]  \hspace{1cm} (2.18)

where \( K_s \) is the maximum value of conductivity, reached in saturated conditions (\( h = 0 \) and \( \theta = \theta_s \)), and \( K_r \) is dimensionless relative conductivity, expressed as function of either saturation or pressure head (for simplicity of presentation we assume here that the hydraulic conductivity is a scalar). Fig. 2.2b presents relative conductivity curves for three different soil textural classes according to Carsel & Parrish (1988). The values of saturated conductivity are: \( K_s = 29.7 \) cm/h for sand, \( K_s = 1.02 \) cm/h for loam and \( K_s = 0.2 \) cm/h for clay.

The mathematical models of relative conductivity are often related to the models of retention function. Theoretical considerations based on the conceptualization of microscopic flow in the pores were applied by Childs & Collis-George (1950), Burdine (1953) and Mualem (1976) to derive expressions for \( K_r \). The models of Burdine and Mualem can be written in the following generalized form (Kosugi et al., 2002):

\[ K_r = S^\tau \left[ \frac{\int_0^{S_e} h^{-\beta} dS}{\int_0^1 h^{-\beta} dS} \right]^\gamma \]  \hspace{1cm} (2.19)

where \( \tau \), \( \beta \) and \( \gamma \) are parameters related to the tortuosity of pores. In the original model of Burdine \( \tau = 2 \), \( \beta = 2 \) and \( \gamma = 1 \), while in the model of Mualem \( \tau = 0.5 \), \( \beta = 1 \) and \( \gamma = 2 \). The tortuosity parameter \( \tau \) is often treated as additional fitting parameter (Kosugi et al.,
If the conductivity function (2.19) is combined with Brooks-Corey retention function (2.16) following relation results:

\[
K_r = S_e^{\eta} \quad h < h_a \tag{2.20}
\]
\[
K_r = 1 \quad h \geq h_a \tag{2.21}
\]

where \(\eta = \tau + 1 + 2/\lambda\) for Burdine’s model, \(\eta = \tau + 2 + 2/\lambda\) for Mualem’s model or \(\eta\) is treated as an independent fitting parameter.

The van Genuchten retention function (2.17) with \(m = 1 - 1/n\) inserted into (2.19) (Mualem’s hypothesis) gives the following expression:

\[
K_r = S_E^{0.5} \left[ 1 - \left( 1 - S_E^{1/m} \right)^m \right]^2 \tag{2.22}
\]

or:

\[
K_r = \frac{\left( 1 - (\alpha|h|)^{n-1} [1 + (\alpha|h|)^n]^{-m} \right)^2}{[1 + (\alpha|h|)^n]^{m/2}} \tag{2.23}
\]

The van Genuchten – Mualem functions (2.17) and (2.22) are one of the most popular model for the constitutive relationships.

The mathematical description of the retention and conductivity curve is further complicated by the presence of hysteresis. Generally, for a specific pressure head the water content is greater during drainage than during wetting. This behavior is caused by the presence of entrapped air, by the ink-bottle effect and by the fact, that the wetting angle is different for advancing and receding wetting front (Kutilek & Nielsen, 1994). Thus, the hydraulic functions are not unique and depend on the history of flow (wetting-drainage cycles).

### 2.3 Modeling of unsaturated flow at the macroscopic scale

The Richards equation (2.10) together with the retention and conductivity functions form the complete flow model at the local (Darcy) scale. At this scale most natural porous media are heterogeneous, which means that their hydraulic properties vary in space. If the number of heterogeneities in the solution domain is not very large the local geometry can be explicitly represented on the numerical grid and the equation is solved directly at the local scale. In many cases the domain of interest includes very large number of heterogeneities. This is especially true for double-porosity soils. In such situations the direct simulation would require excessively large grid. The contrasting values of hydraulic parameters of the highly and weakly conductive porous regions cause additional problems in numerical
integration. Although the numerical methods and the computer capabilities are constantly being improved, at present such type of problems remains intractable from the practical point of view. This fact motivates the development of the macroscopic models, where the heterogeneous medium is replaced by its homogenized equivalent, characterized by some effective parameters.

Generally, one can distinguish two major approaches to the macroscopic description of the flow. The first one is often referred to as the phenomenological approach. The models are introduced directly at the macroscopic scale and their form is proposed on the basis of some empirical considerations. A large group of models is based on the assumption that the large-scale equation has the same form as local-scale flow equation. The focus is directed to the estimation of the macroscopic (effective) parameters (Renard & de Marsily, 1997). Such methods can be very inaccurate when the flow is dominated by the non-equilibrium effects. Thus, another group of proposed models includes various empirical non-equilibrium mechanisms e.g. (Gerke & van Genuchten, 1993a; Ross & Smettem, 2000).

The second approach concerns up-scaling methods which allow mathematically rigorous derivation of the macroscopic scale equations from the description of the physical process at the local scale (Hornung, 1997; Whitaker, 1999). The resulting macroscopic equations may be very different from the local-scale equations. The passage from the local scale to the macroscopic scale can be performed using different mathematical techniques. Two methods which are currently widely used for modeling flow in porous media are the homogenization method and the volume averaging method.

The homogenization method can be defined as asymptotic analysis for periodic media. The principles of this method can be found in the works of Bensoussan et al. (1978) and Sanchez-Palencia (1980). Auriault (1983, 1991) proposed an approach which can be called physical homogenization. He puts emphasis on the analysis of dimensionless numbers governing the physical process. In this way one can identify the situations for which homogenization is not possible and precisely define the domain of validity of the obtained macroscopic models. No assumptions on the final form of the macroscopic model are made. Numerous applications of homogenization concerning porous media mechanics can be found in literature (Hornung, 1997; Mei et al., 1997). In our study the homogenization technique proposed by Auriault (1991) will be used to derive macroscopic description of unsaturated flow in highly heterogeneous double-porosity media. Thus, more details on this method are presented in Chapter 3.

The volume averaging method is in many aspects similar to the asymptotic homogenization, although it employs different mathematical formulation. A comparison of the two approaches can be found in the paper by Bourgeat et al. (1988). It has been used by nu-
merous authors for modeling transfer phenomena in porous media (Bear, 1972; Bachmat & Bear, 1991, among others). In recent years the formalism of the volume averaging method has been substantially developed (Whitaker, 1999) and applied to various problems including single-phase (Quintard & Whitaker, 1987) and two-phase flow (Quintard & Whitaker, 1988) and miscible transport (Quintard et al., 2001). The derivation of the equations describing the process at a larger scale is performed by taking the volume average of the governing equations from a smaller scale. Various levels of averaging are possible. The local volume averaging is used for passing from the pore scale to the Darcy (local) scale (Whitaker, 1986). The resulting equations can be successively up-scaled using the large-scale averaging technique (Quintard & Whitaker, 1987, 1988). The large-scale equations are written in terms of averaged (macroscopic) variables. The local variables are represented as a sum of the averaged value and the spatial deviation. The averaged large-scale equations should be completed by the relations between the averaged values and their local scale deviations. These relations are given by differential equations which constitute the closure problem. Solution of the closure problem allows to obtain the large-scale effective parameters of the system.

One should note that the up-scaling methods may lead to macroscopic models which have the same form as the models proposed on the phenomenological basis. However, the main advantage of the mathematically rigorous up-scaling techniques is that they provide sound theoretical background for the developed models and the answer to the following questions:

- does the equivalent macroscopic model exist?
- what is the form of the macroscopic model?
- how to define the effective parameters of the medium?
- what is the domain of validity of the derived models?

All those issues are comprehensively addressed in the framework of the up-scaling methods.

In the following sections we shall briefly present some models of flow in heterogeneous soils and rocks, which are proposed in the literature. We shall focus mostly on the results concerning the unsaturated water flow, where the Richards assumption is applicable. However, one should note that similar macroscopic models were studied also in the context of saturated water flow (Hornung, 1997; Renard & de Marsily, 1997; Wen & Gómez-Hernández, 1996, e.g.) or two-phase flow (Hornung, 1997; Barker & Thibau, 1997, e.g.).

The available models concern three distinct classes of heterogeneous porous media:

1. moderately heterogeneous media, where the difference in the hydraulic properties of the components is not very large;
2. double-porosity media, consisting of a highly conductive interconnected sub-domain and weakly conductive regions (interconnected or disconnected);

3. double-porosity media consisting of weakly conductive porous matrix with highly conductive disconnected porous inclusions.

Special attention will be directed to the second class of media, where the flow reveals non-equilibrium character. We present various attempts to capture this effects, either on the phenomenological basis or using the up-scaling methods.

2.3.1 Moderately heterogeneous media

Moderately heterogeneous soils are composed of regions characterized by different, but not contrasting hydraulic parameters. When the conductivity of the components is of similar order, one can assume local equilibrium of pressure during the flow. In the framework of the phenomenological approach it is assumed that the macroscopic equation has similar form as the local-scale Richards equation, with the effective parameters representing averaged large-scale properties of the medium. The effective parameters for unsaturated and two-phase flow can be estimated using various techniques like renormalization (King, 1989; Renard, 1997), effective medium theory (Dagan, 1989; Ibraim et al., 2002) and stochastic analysis (Mantoglou & Gelhar, 1987c,a,b; Yeh et al., 1985a,b,c). In the petroleum engineering the pseudo functions are widely used (Jacks et al., 1973; Kyte & Berry, 1975; Stone, 1991; Hewett & Yamada, 1997). They provide equivalent large-scale relation between saturation, relative permeability and capillary pressure.

The macroscopic behavior of moderately heterogeneous porous media was also studied using asymptotic homogenization method. Models for single-phase flow (Saez et al., 1989), two-phase flow (Saez et al., 1989; Bourgeat, 1997) and unsaturated flow (Lewandowska & Laurent, 2001) are available in the literature. Recently, Lewandowska & Laurent (2000, 2001) applied the homogenization technique proposed by Auriault (1991) to study water transfer in heterogenous porous media in the unsaturated conditions. They analyzed flow in a medium composed of two distinct sub-domains. At the local scale, the flow was governed by the Richards equation in both sub-domains. It was assumed that the hydraulic parameters (capillary capacity and hydraulic conductivity) of the two components are of the same order of magnitude. This assumption led to an equilibrium model. The resulting macroscopic model was characterized by a single macroscopic pressure field and two macroscopic water content (saturation) fields (the retention functions can be different for each sub-domain). It was found that the effective capillary capacity depends on the local capacities of the two regions and on their volume fractions. The effective conductivity depends on the conductivities...
of the two components. It is obtained from the solution of a local boundary value problem over the domain of a single period (REV). The problem is given by an elliptic equation with periodic boundary conditions. The solution has form of a vector function, which appears in the definition of the effective conductivity. It represents the influence of the local geometry on the macroscopic transfer properties of the medium. A method for iterative calculation of the effective capacity and effective conductivity was provided.

The results obtained by Lewandowska & Laurent (2001) can be compared to other studies of single-phase and two-phase flow in moderately heterogenous media. The analysis by the homogenization method (Saez et al., 1989) and by the volume averaging method (Quintard & Whitaker, 1987, 1988) showed that for the local equilibrium conditions the macroscopic model has the form of a single equation with effective parameters. The effective conductivity (or permeability) of the medium is obtained from the solution of the local boundary value problem (Saez et al., 1989) or closure problem (Quintard & Whitaker, 1987, 1988) which are equivalent to the formulation of Lewandowska & Laurent (2001). The analysis was extended to the random porous media by Ahmadi & Quintard (1996).

Similar macroscopic models were obtained using the reduced pressure model (Chavent & Jaffre, 1986), widely applied in petroleum engineering. Amaziane et al. (1991) presented a macroscopic two-phase flow model for a medium composed of two sub-domains characterized by the same capillary pressure — saturation function, but having different permeability. The obtained macroscopic equation written in terms of the reduced pressure can be treated as analogue of the models proposed by Saez et al. (1989) or Lewandowska & Laurent (2001). The local equilibrium exists and the effective permeability is obtained from the local boundary value problem. The results were further extended to the case of different capillary pressure functions (Bourgeat & Hidani, 1995). A general homogenized model based on the reduced pressure formulation was presented by Bourgeat (1997). The model is complex due to the coupling of macroscopic and local variables, but it can be simplified in some particular cases.

### 2.3.2 Double-porosity media with highly conductive regions interconnected

In this section we examine models for flow in the double-porosity soils, i.e. soils which are composed of two sub-domains with contrasting hydraulic parameters. The highly conductive regions form an interconnected system, which contributes significantly to the flow. Typical examples of such media are aggregated or macroporous soils.
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Composite hydraulic functions

Various models for double-porosity soils were proposed on the phenomenological basis — a comprehensive review can be found in the paper of Šimůnek et al. (2003). In the vadose zone modeling composite hydraulic functions are often used (Othmer et al., 1991; Durner, 1994; Peters & Klavetter, 1988; Smettem et al., 1991; Šimůnek et al., 1998). They allow to account for rapid changes of the soil properties in the near-saturation region, which is caused by the presence of macropores. The macropores become activated when the capillary pressure tends to 0 (full saturation). The medium is conceptualized as two or more overlapping regions (e.g. macropores, mesopores and micropores). Each region is characterized by its own pore size distribution and hydraulic functions. The characteristic of entire bi-modal or multi-modal system is obtained by the linear superposition of the local functions. Durner et al. (1999) used a combination of the van Genuchten type functions for each regions. Other authors used linear (Vogel & Císlarová, 1988) or exponential (Mohanty et al., 1997) conductivity functions in the near-saturation range. Note however that such approach does not introduce any non-equilibrium mechanism and thus cannot reproduce the typical double-porosity effects.

Model of Ross & Smettem (2000)

A relatively simple non-equilibrium model has been proposed by Ross & Smettem (2000). They combined the Richards equation with an additional relation describing the dynamics of water content:

$$ \frac{\partial \theta}{\partial t} = f(\theta, \theta_e) = \frac{\theta_e - \theta}{\tau} \quad (2.24) $$

where $\theta_e$ is the soil water retention function corresponding to the equilibrium conditions and $\tau$ is an equilibration time constant. An advantage of such model is that it requires only one additional parameter compared to the classical Richards equation. The parameter $\tau$ however has no clear physical interpretation.

Phenomenological double-porosity models

The non-equilibrium flow in double-porosity media is commonly described using the two-equation approach initially introduced by Barenblatt et al. (1960) for the description of fractured reservoirs. In their model the porous formation consists of two overlapping sub-domains. One sub-domain is associated with the more conductive system of fractures, while the other sub-domain represents the weakly conductive porous blocks. Each system is characterized by its own set of macroscopic variables and hydraulic parameters. The flow in each region is described by a separate equation. The equations are coupled by a transfer term describing the water exchange between the sub-domains. This type of two-equation models
has been extensively used in recent decades to describe single-phase, two-phase and unsaturated flow as well as the contaminant transport in double-porosity soils and rocks (Bear et al., 1993; Chen, 1989; Šimůnek et al., 2003). Several variants of this approach have been developed, which may be classified according to different criteria. Those criteria include the contribution of the two sub-domains to the flow process, the form of the equation describing flow in the more conductive sub-domain and the form of the exchange term.

As far as the contribution of the two regions to the macroscopic flow in considered, three types of the model can be distinguished. In the most general form (Barenblatt et al., 1960; Gerke & van Genuchten, 1993a) two macroscopic equations are assumed to describe flow in fractures and blocks. Another model results when the blocks are assumed to be disconnected and/or very weakly conductive. The macroscopic flow takes place in the highly conductive interconnected sub-domain and the blocks acts only as a source/sink term (Warren & Root, 1963). In the simplest form it is assumed that the volume fraction of fractures is so small that they have no storage capacity and consequently the retention term in the equation for fractures is neglected (Barenblatt, 1963). In many recent publications (Jarvis, 1998; Šimůnek et al., 2003) the term dual-porosity is used for the second and third type of models, while the first type is referred to as dual-permeability models.

In most of the two-equation models developed for unsaturated soils the flow in weakly conductive matrix blocks or soil aggregates is described by the Richards equation. In contrast, the more conductive sub-domain may consist of a network of large fissures or macropores and various mathematical formulation of flow in this region were proposed. They include Poisseeul’s equation (Ahuja & Hebson, 1992), the Green and Ampt infiltration model (Ahuja & Hebson, 1992; Chen & Wagenet, 1992), the kinematic wave equation (Jarvis, 1994) and the Richards equation (Gerke & van Genuchten, 1993a; Zimmerman et al., 1996). In the latter case modification of the standard models of retention and conductivity functions are available, which can be applied for flow in fractures (Kwicklis & Healey, 1993; Liu & Bodvarsson, 2001, among other).

Another important aspect of the double-porosity models is the representation of the water transfer between the two sub-domains. The most widespread formulation, proposed by Warren & Root (1963), relates the water transfer directly to the difference in pressures between the sub-domains. Such approximation is relatively accurate for quasi-steady state, but it fails to represent highly transient flow, for example at the initial stages of the infiltration. Other, more accurate formulation expressed in terms of the two pressures has also been proposed (Dykhuizen, 1990; Zimmerman et al., 1993). Alternatively, the transfer rate may be related to the difference in saturations of the two regions (Jarvis, 1994; Šimůnek et al., 2003). One should note that the transfer term approximations have been initially developed for linear
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problems: diffusion or saturated flow. For this type of problems numerous solutions are available (Barker, 1985; Auriault & Lewandowska, 1995; Royer et al., 1996; De Swann, 1976, among others). However, their extension to the nonlinear problems of unsaturated flow is not necessarily straightforward. Finally, instead of using averaged macroscopic variables, the exchange term can be obtained from the direct solution of local flow in weakly conductive aggregates / blocks. Pruess & Narasimhan (1985) developed a multiple interacting continua model. In this approach matrix blocks are divided into nested sub-grids to accommodate slow changes in local variables, which varies in function of the distance from fracture.

Model of Gerke & van Genuchten (1993a)

Gerke & van Genuchten (1993a) proposed the following double-permeability model based on the Richards equation:

\[ C_1 \frac{\partial h_1}{\partial t} - \nabla \cdot (K_1 \nabla (h_1 + X_3)) + \frac{Q}{w_1} = 0 \]  \hspace{1cm} (2.25)

\[ C_2 \frac{\partial h_2}{\partial t} - \nabla \cdot (K_2 \nabla (h_2 + X_3)) - \frac{Q}{w_2} = 0 \]  \hspace{1cm} (2.26)

where \( w, C, K, h \) denotes respectively the volume fraction, specific water capacity, hydraulic conductivity (scalar) and capillary pressure head of the two sub-domains. Subscript 1 refers to the highly conductive system and subscript 2 to the weakly conductive system. The macroscopic (bulk) soil properties are given by the following relations:

\[ \theta = w_1 \theta_1 + w_2 \theta_2 \]  \hspace{1cm} (2.27)

\[ q = w_1 q_1 + w_2 q_2 \]  \hspace{1cm} (2.28)

\[ K = w_1 K_1 + w_2 K_2 \]  \hspace{1cm} (2.29)

where \( \theta \) is the average volumetric water content, \( q \) is the macroscopic flux and \( K \) is the macroscopic hydraulic conductivity. One should note that such estimation of the macroscopic conductivity holds only for simple geometries (i.e. layers parallel to the flow direction).

The water transfer term is given by the following first-order expression:

\[ Q = \frac{\beta}{a^3 \gamma_w} K_a(h) (h_1 - h_2) \]  \hspace{1cm} (2.30)

where \( \beta \) is a dimensionless geometry-dependent coefficient, \( a \) is the characteristic length of weakly conductive structure (block or aggregate), \( \gamma_w \) is a dimensionless scaling factor and \( K_a(h) \) is the conductivity at the interface. The interface conductivity may be equal to the conductivity of blocks or may assume smaller values, for example due to the skin effect. Gerke & van Genuchten (1993b) tested various methods of evaluation of the interface
conductivity and they proposed the following formula:

$$K_a = \frac{1}{2} (K_a(h_1) + K_a(h_2))$$ (2.31)

as the most practical approximation. The authors also derived the value of the scaling factor \(\gamma_w = 0.4\), which ensured best agreement with the results of direct numerical simulation of diffusive flow in a slab-like matrix block. The coefficient \(\beta\) is closely related to the normalized surface to volume ratio \(\zeta\) characterizing the porous blocks (Gerke & van Genuchten, 1996):

$$\zeta = \frac{A^*}{V^* a^*}$$ (2.32)

where \(A^*, V^*, a^*\) denote the effective surface area, the volume and the effective length of the considered aggregates or blocks (\(\zeta = 3\) for spheres, 2 for cylinders and 1 for slabs). Gerke & van Genuchten (1996) provided an empirical description of this relation:

$$\beta = \begin{cases} 
0.19 \ln \left( \frac{2}{\zeta} - 1 \right) & 0.0198 < \zeta < 1 \\
3.6 \zeta^{1.5} & 1 \leq \zeta \leq 2 \\
11.4275 - 7.4438\zeta + 3.5473\zeta^2 & 2 < \zeta \leq 10 
\end{cases}$$ (2.33-2.35)

A simplified version of the model (2.25)–(2.26) also appears in the literature (Šimůnek et al., 2001, 2003), where the blocks act only as a source term and the equation (2.30) becomes:

$$w_2C_2 \frac{\partial h}{\partial t} = \omega(S_{e1} - S_{e2})$$ (2.36)

In the source term appearing at the right-hand side of equation \(\omega\) is an empirical constant coefficient and \(S_{e1}\) and \(S_{e2}\) are the effective saturations of the highly and weakly conductive sub-domains respectively. The transfer rate is proportional to the difference in saturation. Such approach reduces the number of parameters required by the model, but it seems to be less realistic, since the retention curve is assumed the same for both regions.

**Model of Zimmerman et al. (1996)**

Zimmerman et al. (1996) presented a dual-porosity model for the unsaturated flow in fractured rocks:

$$m_1 \frac{\partial S_1}{\partial t} - \nabla \cdot \left[ \frac{k_1 k_{r1}}{\mu} \nabla (p_1 + \rho g X_3) \right] + Q = 0$$ (2.37)

where \(k\) is the absolute permeability, \(k_{r1}\) is the relative permeability of the fracture continuum, \(\mu\) is the dynamic viscosity of water, \(p\) is the potential of water in fractures, \(\rho\) is the density of water, \(g\) is the gravitational acceleration, \(m_1\) is the fracture porosity and \(S_1\) is the saturation of the fracture continuum. \(Q\) represents instantaneous volumetric flux between fractures
and blocks. Zimmerman et al. (1996) discusses various available formulations of the transfer term in context of the unsaturated flow. The Warren & Root (1963) approximation is given by:

\[ Q = \frac{\alpha (1 - m) k_2 k_r^2}{\mu} (p_2 - p_1) \]  

(2.38)

As it has been mentioned, it produces inaccurate results for short times. An improved formula for short times was proposed by Dykhuizen (1990):

\[ Q = \frac{-\alpha (1 - m) k_2 k_r^2 (p_1 - p_i)^2}{\mu \cdot 2 (p_2 - p_i)} \]  

(2.39)

Finally, Zimmerman et al. (1996) used the Vermeulen’s approximation:

\[ Q = \frac{\alpha (1 - m) k_2 k_r^2 (p_2 - p_i)^2 - (p_1 - p_i)^2}{2 (p_2 - p_i)} \]  

(2.40)

It was shown that this formula gives satisfying results for short and long times.

**Model of Jarvis (1994)**

Another possible approach is to use the *kinematic wave equation* suggested by Germann (1985) and Germann & Beven (1985) to simulate flow in the more conductive system of fissures or macropores. It has been applied for example in the MACRO model (Jarvis, 1994). The governing equations are:

\[ \frac{\partial \theta_1}{\partial t} + \frac{\partial}{\partial X_3} \left[ K_{s1} \left( \frac{\theta_1}{\theta_{s1}} \right)^b \right] + Q = 0 \]  

(2.41)

\[ C_2 \frac{\partial h}{\partial t} - \nabla \cdot (K_2 \nabla (h + X_3)) - Q = 0 \]  

(2.42)

where \( \theta_1 \) and \( \theta_{s1} \) are the actual and saturated water content in the macropores, \( K_{s1} \) is the saturated hydraulic conductivity of the macropores and \( b \) is an empirical parameter characterizing the macropores. The transfer term \( Q \) is proportional to the difference in water content:

\[ Q = \frac{\beta D_w \gamma_w}{a^2} (\theta_{s2} - \theta_2) \]  

(2.43)

where \( D_w \) is the effective water diffusivity, \( \theta_{s2} \) and \( \theta_2 \) are the saturated and actual water content in the micropore sub-domain. The advantage of this model is that it requires fewer parameters than the models based entirely on Richards equation, since no retention curve is needed for the macropore region. On the other hand, its application is limited to the vertical gravitational flow. Neither horizontal nor upward preferential flow can be modeled. Nevertheless the MACRO model has been widely used in field studies. Note that equation (2.43) includes no dispersive mechanism. To account for dispersive effects an improved version of the model has been proposed, known as *kinematic-dispersive wave* (Di Pietro et al., 2003).
Multi-porosity models

The concept of dual structure can be also extended for the situations when more than two distinct porous regions are presented (Gwo et al., 1995; Hutson & Wagenet, 1996). Gwo et al. (1995) developed a conceptual model of three overlapping porous regions, corresponding to macropores, mezopores and micropores, respectively. It was assumed that the flow in each sub-domain is described by Richards equation and the transfer rate between sub-domains by a first order approximation. The mass exchange is allowed between all regions and is described by a first order approximation.

Model of Hornung (1991)

The non-equilibrium flow has been also studied using rigorous up-scaling methods. However, most of the applications concerned either two-phase incompressible flow or slightly compressible single-phase flow. The unsaturated flow has been specifically addressed by Hornung (1991). The starting point for the analysis was the local-scale Richards equation in the two porous regions. The resulting macroscopic model has complex form. At the macroscopic scale the flow is driven by the capillary and gravity forces. It is described by a single equation with highly nonlinear source term, representing the interaction between the highly and weakly conductive sub-domains. In order to obtain values of the source term one has to solve local-scale flow equation in a representative aggregate (block) at each point of the macroscopic domain. Thus, the macroscopic and local variables are coupled. It has been shown that the effective conductivity depends only on the local conductivity of the more conductive region and on the local geometry. It is obtained from the solution of a local boundary value problem, which is defined over the more conductive part of the period. The effective capillary capacity was shown to depend on the local capacity of the highly conductive region and its volume fraction.

Other models

One-equation models were obtained by Arbogast et al. (1990) and Douglas & Arbogast (1990) for single-phase flow and two-phase flow in fractured media. In each case the macroscopic model consists of a single equation, with effective parameters corresponding to the highly conductive fracture sub-domain. The influence of blocks is represented by a highly nonlinear source term. In the models of Arbogast et al. (1990) and Hornung (1991) the local flow in blocks is not affected by gravity. The gravity at the local scale has been included in modified models presented by Arbogast (1993a, b).

The two-equation formulation has been also obtained using up-scaling methods, however
the available contributions concern linear single-phase flow. Douglas et al. (1997) proposed a model for partially fissured media, where the flow between weakly conductive blocks is also accounted for. In this case two macroscopic equations were obtained. In addition, the flow in blocks is represented by local scale equations, used to calculate the exchange rate between the two sub-domains. Quintard & Whitaker (1996) derived a model for single-phase quasi-steady flow. It consists of two equations describing evolution of region-averaged pressures. The exchange between regions is directly proportional to the difference in pressures, which is consistent with the Warren and Root formula (Warren & Root, 1963). The effective permeability for each region and the transfer coefficient appearing in coupling term are calculated from three closure problems, which completes the model. It has been shown (Noetinger et al., 2001b) that the same values of effective coefficients are obtained with the continuous time random walk method (Noetinger et al., 2001a), based on the particle-tracking.

Quintard & Whitaker (1990a,b) extended their two-phase flow analysis (Quintard & Whitaker, 1988) for the dynamic case, when the pressure gradients and the transient effects create non-equilibrium effects in the large-scale averaging volume. They examined the case, when the separation of scales is not satisfied. In that case the large-scale properties were shown to depend on the large-scale pressure gradients, the gravity orientation and the time derivative of large-scale saturation and the closure problems become very complex and non-periodic.

Panfilov (2000) used the asymptotic homogenization to develop a general two-phase flow model for heterogenous soils composed of highly conductive connected matrix and weakly conductive blocks. The model accounts for different flow situations, i.e. the source-type flow (Bourgeat & Panfilov, 1998), characterized by radial streamlines in blocks and the translation-type flow, characterized by streamlines in blocks parallel to the direction of the macroscopic flow. In the macroscopic model both the capillary pressure function and the phase permeability functions are dynamic, i.e. they depend on time. The mass exchange between matrix and blocks is related to the values of the macroscopic pressure in the two regions. The capillary relaxation time, which determines the time required to equilibrate the saturation in blocks, is defined from the solution of a local boundary value problem and it depends on saturation. An analysis for transient single-phase flow is presented in (Bertin et al., 2000). In the developed model an additional non-equilibrium term appears in the Darcy’s law. The effective permeability tensor is non-stationary and is changing in time. This effect is superposed with another relaxation phenomenon caused by the exchange between the highly and weakly conductive sub-domains. All relaxation parameters are explicitly determined from the solution of local boundary value problems.
2.3.3 Double-porosity media with highly conductive inclusions

While the models for the media with the more conductive sub-domain connected are widely studied in literature, the media with inverse structure receive much less attention. The inverse structure means that highly conductive inclusions are embedded in a porous matrix of low conductivity and they are not connected with each other. The inclusions may be either void (closed fissures or macropores, vugs) or filled with porous material. The macroscopic behavior of such system is very different from the one described above. To our knowledge, only few contributions concerning this problem are available and they are not directly related to the unsaturated flow. Levy (1990) analyzed the saturated flow through non deformable fissured rocks, formed of porous blocks separated from each other by a system of fissures. The homogenization method with multiple scale asymptotic expansions was used to solve the Stokes equations and to obtain the macroscopic filtration law for the stationary and incompressible flow. The influence of the fissures connectivity was emphasized, since two very different macroscopic models are derived in the extreme cases of completely connected fissures or a system of closed fissures.

Panfilov et al. (1997) studied the capillary flow of two immiscible fluid phases in a porous medium with highly conductive inclusions embedded in a weakly conductive matrix. It was assumed that capillarity in inclusions is much lower than in the matrix and the permeability is much higher. Depending on the saturation of the wetting fluid phase in the two regions different situations are distinguished: entirely frozen mode (the wetting phase is immobile in both regions), partially frozen mode (the phase is immobile in inclusions), nonlinear mode and quasi-linear mode (the phase flows in both domains, while the relation between capillary pressure and saturation has nonlinear or quasi-linear character). In all those situations capillary equilibrium conditions are satisfied. The quasi-linear mode of flow is studied using asymptotic homogenization method. It has been proved that the effective two-phase flow does not depend on the relative permeability in the highly conductive inclusions. Theoretical results showed good agreement with the laboratory experiments (Alhanai et al., 1992; Bertin et al., 1997) concerning the displacement of oil by water.

Independently of the derivation of the macroscopic models, numerous papers on the estimation of the effective transfer parameters for media with highly permeable inclusions have been published. For example Moctezuma-Berthier A. (2004) studied the permeability in reconstructed bimodal porous media (vugular media). In the paper by Ibraim et al. (2002) the permeability of isotropic heterogeneous soils is studied by a self-consistent method. Several analytical formulas are derived to calculate the conductivity of soils made of two or three constituents such as saturated clay, impervious grains and perfectly permeable water pockets.
2.4 Numerical implementation of the macroscopic flow models for unsaturated soils

2.4.1 Numerical solution of the macroscopic models

The macroscopic flow models presented in the preceding sections have form of highly non-linear partial differential (or integro-differential) equations. Generally, analytical solutions for such equations are not available and they should be solved numerically. In the following paragraphs we summarize some basic information concerning the numerical algorithms, with focus on the equations based on the Richards assumption. From the numerical point of view the macroscopic models of unsaturated flow can be divided in three groups.

First group includes the macroscopic models which has the same form as the local-scale Richards equation e.g. (Lewandowska & Laurent, 2001). In such case one can use the standard algorithms developed for the unsaturated flow equation, which are extensively discussed in the literature. A general mass conservative scheme has been proposed by Celia et al. (1990) and Rathfelder & Abriola (1994). They used mixed form of Richards equation, with the retention term expressed as the derivative of water content $\frac{\partial \theta}{\partial t}$ rather than the pressure-based form $C \frac{\partial h}{\partial t}$. Such approach significantly improves mass balance. For the discretization in space either finite difference (Haverkamp et al., 1977; Tocci et al., 1997) or finite element (Pan et al., 1996; Šimůnek et al., 1998) methods are routinely used. For finite elements diagonalization of mass matrix is necessary, since the standard Galerkin approach produces oscillations in the solution (Celia et al., 1990; Pan et al., 1996). For the discretization in time the fully implicit scheme (Šimůnek et al., 1998) or the Crank-Nicholson scheme (Fayer, 2000) are commonly used. The resulting discretized equations are linearized using Picard or Newton method. The Picard scheme is easier to implement and seems to be more popular (Šimůnek et al., 1998; Celia et al., 1990). Lehmann & Ackerer (1998) compared the two methods and found the Newton scheme more efficient in terms of the number of time steps and iteration. Another proposition is to use the pressure-based form of equation combined with high-order time discretization schemes. Tocci et al. (1997) and Miller et al. (1998) applied the solver DASPK to the system of ordinary differential equations resulting from spatial discretization of equation (method of lines). The same approach was used by Szymkiewicz & Lewandowska (2002), who developed REMOL-1D code to study sharp-front infiltration in dry soils. Numerical experiments show that this method keeps good mass balance and can reduce required computational effort especially when high accuracy is required. However, in many practical cases it does not show significant advantage over the standard approach. The Richards equation can be also solved using transformation of
variables (Williams et al., 2000). Such approach can significantly relieve problems caused by nonlinearity of hydraulic parameters. Various techniques have been proposed including the water content based transform (Kirkland et al., 1992), Kirchhoff integral transform (Haverkamp et al., 1977), hyperbolic sine transform (Ross, 1990) or rational function transform (Pan & Wierenga, 1995). Papers addressing various aspects of the numerical solution of the unsaturated flow equation include (Haverkamp & Vauclin, 1979; Kavetski et al., 2001; Romano et al., 1998; van Dam & Feddes, 2000; Zhang & Ewen, 2000; Zhang et al., 2002) among many other.

Another group of models is represented by the two-equation double-porosity or double-permeability formulations. Gerke & van Genuchten (1993a) presented numerical implementation of their model. They concluded that for the reasons of stability the two equations should be solved simultaneously. Each equation is discretized in similar manner as the standard Richards equation. The only difference is that in one-dimensional case the resulting matrices of coefficients for one dimensional flow have seven diagonals. In contrast, the numerical method implemented in the MACRO model (Jarvis, 1994) decouples the solution of equations for micropore and macropore regions. The Richards’ equation is solved with an explicit finite difference scheme, while implicit method is used for the kinematic wave equation.

A specific class of models arise from the homogenization procedure for double-porosity media (Hornung, 1991; Arbogast, 1997). The equations have integro-differential form and they are characterized by coupling of the macroscopic and local variables. The solution of local-scale flow in the weakly conductive blocks is required to obtain the values of the source term appearing in the macroscopic equation. Since the flow at both scales can be very unsteady, the source term should be treated implicitly. It means that the local and macroscopic equations should be solved simultaneously in the same iteration. Arbogast (1997) presented a numerical algorithm for similar macroscopic models arising for single-phase and two-phase flow. The numerical scheme was based on fully implicit time discretization and Newton iterative method. Similar concept, although not resulting from homogenization, has been applied in the multiple interacting continua (MINC) models (Pruess & Narasimhan, 1985; Pruess, 1991). Nevertheless, no detailed discussion of such algorithms for unsaturated flow is available and the problem remains challenging for practical application.

2.4.2 Numerical calculation of the effective parameters

Numerical methods should be used to solve the local boundary value problem or the closure problem which result from the homogenization or volume averaging. They define the effective conductivity (or permeability) of the heterogeneous medium. The local boundary value
problem is an elliptic equation in two- or three-dimensional domain with periodic boundary conditions. Such problems can be solved using finite difference, finite element or finite volume method. For example a finite volume code MONO-3D was developed by Quintard (1997) to solve the closure problem resulting from large-scale averaging procedure for single phase flow (Quintard & Whitaker, 1987).

2.5 Experimental investigation of the unsaturated and two-phase flow in the double-porosity media

Application of the theoretical models to describe real situations is the major objective underlying their development. However, in the case of flow in unsaturated double-porosity soils the practical application of theoretical models remains somewhat limited. The main reason is that they require many parameters to be identified. In the ideal situation one should have knowledge about the local geometry and the hydraulic characteristics of the two components of the medium. This is hardly possible in practice and the question arises about identification of the parameters (see Clothier et al., 1995; Jaynes et al., 1995; Schwartz et al., 2000; Köhne et al., 2002a,b; Logsdon, 2002, among others). Inverse techniques are routinely used to estimate at least some of the required parameters. In that case the verification of the model may be difficult, since one cannot distinguish between model errors and parameter errors (Larsson & Jarvis, 1999). Such problems are mentioned in the available papers on the practical application of the double-porosity models.

The experimental verification of the Gerke & van Genuchten (1993a) model was presented by Šimůnek et al. (2001). A series of upward infiltration experiments was performed on undisturbed soil samples. The experimental results were analyzed using three different models: single-porosity equilibrium model, dual-porosity model and dual-permeability model. In each case the effective parameters of the macroscopic model were identified by inverse technique. It was found that the non-equilibrium behavior can be reproduced with reasonable accuracy by both dual-porosity and dual-permeability models, which raise the question about the domain of validity of those models.

Gerke & Köhne (2004) applied the model of Gerke & van Genuchten (1993a) to simulate bromide transport in a tile-drained agricultural field. The parameters characterizing geometry (i.e. the volume fractions of the two sub-domains, the aggregate size and the coefficient $\beta$ in the transfer term were estimated empirically by the examination of the soil structure. The retention data were estimated from desorption experiments and the saturated hydraulic conductivity was measured with a steady-state flux method. Those data were then fitted to bimodal retention and conductivity curves in order to find the characteristics corresponding
to the two sub-domains. The residual water content was determined from an additional experiment in a pressure chamber. The parameters of the solute transport equation were found from column tests. The authors emphasized the difficulty in estimating the two parameters from the transfer term, i.e. the conductivity $K_a$ and the diffusion coefficient at the interface. Those parameters were determined by a calibration procedure (fitting of the simulation results to the observation). Although a good agreement has been achieved, the values of transfer coefficients were much less than one might have expected.

The MACRO model of Jarvis (1994) was applied to a number of lysimeter experiments (Saxena et al., 1994) and field-scale experiments (Villholt & Jensen, 1998; Villholt et al., 1998; Larsson & Jarvis, 1999; Ludwig et al., 1999). In most cases the parameters of the model were obtained partially from independent measurements and partially by calibration technique. Larsson & Jarvis (1999) suggested that the simplified description of interaction between the two sub-domains and the uncertainty of boundary conditions as a source of discrepancy between the observations and simulations. Villholt & Jensen (1998) calibrated their model by using different estimations of mass transfer parameters for early and later times of the process, in the latter case excessively small values were required to keep low exchange rate. The difficulty in estimating the parameters of the exchange term was also reported by Ludwig et al. (1999).

Although not directly related to the unsaturated flow, the experiments presented by Alhanai et al. (1992); Bertin et al. (1993) are interesting, since they represent one of few attempts to validate a macroscopic model obtained by an up-scaling method (volume averaging, in this case). The experiments were performed on two different types of nodular media (sand with sandstone inclusions and sandstone with sand inclusions). The parameters of each material were obtained from independent measurements. The experimental results were compared with numerical simulation using the macroscopic models of Quintard & Whitaker (1988) and Bertin et al. (2000). One should note however, that the double-porosity medium was composed of three periodic cells only, which may rise question about the separation of scales.

### 2.6 Summary

As it can be seen from the presented overview, modeling of the unsaturated flow in heterogeneous soils receives much attention in the literature. The mathematical models can be either introduced directly at the macroscopic scale (phenomenological approach) or derived from the local-scale description (up-scaling methods).

In the framework of the phenomenological approach various models have been proposed,
which differ in the complexity of the mathematical formulation and the number of parameters. The phenomenological models are widely used in practice. Nevertheless, a question may arise about their theoretical background.

On the other hand the up-scaling methods enable to develop macroscopic models in a rigorous manner. It seems that their application by now has been focused mostly on the problems of groundwater engineering (single-phase flow) and petroleum engineering (two-phase incompressible or slightly compressible flow). The contributions dealing specifically with the problems of the unsaturated zone are far less numerous.

Practical application of the available theoretical models requires the use of numerical methods. It should be noted that the macroscopic equations often have more complicated form than the Richards equation. In case of non-equilibrium models obtained by homogenization macroscopic and local variables are coupled. Although some suggestions concerning numerical implementation of such models have been presented in the literature, it seems that the problem requires more detailed analysis.

Finally, an overview of the contributions related to the experimental investigation of flow in double-porosity soils reveals several important points. Although a number of laboratory and field tests has been performed, only few of them were actually attempted to validate the theoretical models. Thus the available data cannot be readily used for this purpose. A common problem concerns the determination of parameters, which requires the knowledge of the local geometry and the hydraulic characteristics of the two sub-domains, which are hardly available in the field. Thus, it seems that tests in controlled laboratory conditions are necessary for the comparison with theoretical results.
Chapter 3

Development of the macroscopic models for the unsaturated water flow by homogenization

3.1 Presentation of the method

The theory of asymptotic homogenization is based on two essential assumptions:

1. The medium is periodic. Although this assumption may appear limiting, it allows the use of robust mathematical techniques available for periodic media. On the other hand, the periodicity condition implies the existence of a representative elementary volume at the local scale, which is a necessary assumption for the development of the macroscopic model. It has been shown that the results obtained for periodic media are equivalent to the results obtained for stochastically homogeneous media (Auriault, 2001), thus the periodicity assumption is not restrictive.

2. The local scale and the macroscopic scale are separated from each other. It means that the following condition is satisfied:

\[ \epsilon = \frac{l}{L} \ll 1 \]  

(3.1)

where \( \epsilon \) is the scale parameter, \( l \) is the characteristic length of the period, and \( L \) is characteristic length of the considered macroscopic domain or the macroscopic physical process (Auriault, 2001). The separation of scales is the necessary and fundamental condition for the derivation of the macroscopic models with intrinsic effective parameters. It is the underlying hypothesis in the homogenization theory as well as in the volume averaging method (Quintard & Whitaker, 1987). Homogenization can also be
applied for media showing more than two observation scales, provided that those scales are separated from each other.

The considered physical problem is written in terms of dimensionless variables. Each physical (dimensional) variable $\phi$ is represented as a product of the dimensionless variable $\phi^*$ and the characteristic constant value $\phi^c$:

$$\phi = \phi^* \phi^c \quad (3.2)$$

The separation of scales allows introduction of the two-scale formulation. The dimensional space variable $X$ is replaced by two dimensionless space variables:

- macroscopic variable $x$
- local variable $y$

Those variables satisfy the following relations:

$$x = \frac{X}{L} \quad y = \frac{X}{l} \quad (3.3)$$

$$x = \varepsilon y \quad y = \frac{x}{\varepsilon} \quad (3.4)$$

The homogenization theory postulates that the dimensionless variables can be represented in a form of the following asymptotic expansions:

$$\phi^*(x, y, t^*) = \phi^{*(0)}(x, y, t^*) + \varepsilon \phi^{*(1)}(x, y, t^*) + \varepsilon^2 \phi^{*(2)}(x, y, t^*) + \ldots \quad (3.5)$$

where the successive terms $\phi^{*(i)}(x, y, t^*)$ are $y$-periodic.

The general outline of the homogenization procedure according to Auriault (1991, 2001) is as follows:

1. Description of the physical process at the local scale

2. Normalization of equations. The physical variables are divided by their characteristic values. The physical spatial variable is replaced by the dimensionless local spatial variable $y$.

3. Estimation of the arising dimensionless numbers. Their order of magnitude is assessed with regard to the scale parameter $\varepsilon$. The estimation

$$R = O(\varepsilon^p) \quad (3.6)$$

means that following relation is satisfied:

$$\varepsilon^{p+1} \ll R \ll \varepsilon^{p-1} \quad (3.7)$$

where $R$ is the considered dimensionless number and $p$ is an integer power exponent. The dimensionless numbers in equations are replaced by appropriate powers of $\varepsilon$. 

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4. Introduction of the asymptotic expansions (3.5) into the normalized equations. The spatial derivative operators are replaced by their two-scale equivalents:

$$\frac{\partial}{\partial y} \rightarrow \frac{\partial}{\partial y} + \varepsilon \frac{\partial}{\partial x}$$  (3.8)

5. Identification of the terms at the same power of $\varepsilon$. At each power of $\varepsilon$ a corresponding boundary value problem will arise. Successive solution of those problems allows to derive the macroscopic equation and the effective parameters.

The principal advantages of the homogenization approach are:

- physical and mathematical rigorousness,
- capability of multi-scale analysis,
- derivation of the macroscopic equations without a priori assumptions on their form,
- definition of the intrinsic effective parameters,
- definition of the domain of validity of the macroscopic model.

In the following sections the method of homogenization will be used to derive the macroscopic model of unsaturated water flow from the description at the local scale. The homogenization procedure results in the governing equation at the macroscopic scale, the effective parameters of the medium and the domain of validity of the obtained models.

3.2 Formulation of the problem

3.2.1 General assumptions

We consider the unsaturated water flow in a rigid double-porosity soil. The soil is composed of two sub-domains with contrasting hydraulic properties. We assume that the medium has periodic structure and that the separation of scales (3.1) is satisfied. In the following part the period domain will be denoted by $\Omega$, the more conductive and the less conductive sub-domains of the period by $\Omega_1$ and $\Omega_2$, respectively, and the interface between the two sub-domains by $\Gamma$ (see Fig. 3.1). The volumetric fractions of the more conductive ($w_1$) and the less conductive ($w_2$) sub-domain are of the same order of magnitude:

$$\mathcal{O}(w_1) = \mathcal{O}(w_2)$$  (3.9)

In the following sections two different types of local geometry are considered:
Figure 3.1: Structure of the double-porosity soil at the local scale: (a) weakly conductive inclusions in a highly conductive matrix, (b) highly conductive inclusions in a weakly conductive matrix.

- weakly conductive inclusions embedded in a highly conductive matrix (Fig. 3.1a), studied by Lewandowska et al. (2004b);

- highly conductive inclusions embedded in a weakly conductive matrix (Fig. 3.1b), presented after Lewandowska & Auriault (2004) and Lewandowska et al. (2004a).

As it will be shown, different macroscopic models are obtained for each structure.

We assume that the Richards equation is valid in both sub-domains. The assumptions underlying this equation were presented in Chapter 2. Thus, our analysis does not refer directly to the fractured media, where the highly conductive system of fractures occupy relatively small fraction of space and the flow within this region often does not have capillary character. The models presented below are more relevant to the aggregated soils, shaled sandstones or other formations having two porous components of very different characteristics.
Chapter 3. Development of the macroscopic models by homogenization

3.2.2 Description of flow at the local scale

We assume that at the scale of a single period the unsaturated water flow in each sub-domain is described by the mass balance equation in the form proposed by Richards (1931):

\[ C_1 \frac{\partial h_1}{\partial t} - \frac{\partial}{\partial X_i} \left[ K_{1ij} \frac{\partial}{\partial X_j} (h_1 + X_3) \right] = 0 \quad i, j = 1, 2, 3 \quad \text{in } \Omega_1 \tag{3.10} \]

\[ C_2 \frac{\partial h_2}{\partial t} - \frac{\partial}{\partial X_i} \left[ K_{2ij} \frac{\partial}{\partial X_j} (h_2 + X_3) \right] = 0 \quad \text{in } \Omega_2 \tag{3.11} \]

where \( t \) is time, \( X \) is spatial variable (\( X_3 \) axis is oriented positively upwards), \( C \) is the capillary capacity, \( K \) is the hydraulic conductivity tensor and \( h \) is the water pressure head. The indices 1 and 2 refer to the more conductive sub-domain and the less conductive sub-domain, respectively. The term \( X_3 \) represents the gravity potential. At the interface \( \Gamma \) the pressure head and the flux are continuous:

\[ h_1 = h_2 \quad \text{on } \Gamma \tag{3.12} \]

\[ \left[ K_{1ij} \frac{\partial}{\partial X_j} (h_1 + X_3) \right] N_i = \left[ K_{2ij} \frac{\partial}{\partial X_j} (h_2 + X_3) \right] N_i \quad i, j = 1, 2, 3 \quad \text{on } \Gamma \tag{3.13} \]

where \( N \) is the unit normal vector oriented outward to \( \Omega_2 \). We assume that the hydraulic characteristics of the two regions are known:

\[ C_1 = C_1(h_1) \quad K_1 = K_1(h_1) \tag{3.14} \]

\[ C_2 = C_2(h_2) \quad K_2 = K_2(h_2) \tag{3.15} \]

The capillary capacities \( C_i \) are defined as the slopes of the retention curves \( \theta_i(h_i) \):

\[ C_i = \frac{d\theta_i}{dh_i} \quad i = 1, 2 \tag{3.16} \]

where \( \theta_i \) is the volumetric water content. The functions \( C_i(h_i) \) and \( K_i(h_i) \) are highly nonlinear (see Chapter 2). Due to the diffusive character of the Richards equation the transfer properties of each medium can be characterized by another parameter — the hydraulic diffusivity \( D(h) \):

\[ D_i(h_i) = \frac{K_i(h_i)}{C_i(h_i)} \quad i = 1, 2 \tag{3.17} \]

As it will be shown, the hydraulic diffusivity has fundamental importance in the estimation of the local pressure gradient.

In the following analysis the hysteresis in retention and conductivity curves is neglected. This assumptions is not limiting since when the hysteresis effects are present different functions can be used for the wetting and drying branch. The equations (3.10)–(3.13) with relations (3.14)–(3.15) form the complete description of unsaturated water flow at the local scale.

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3.2.3 Normalization

Each physical variable $\phi$ appearing in equations (3.10)–(3.13) can be represented as a product of a dimensionless variable and a dimensional characteristic constant, according to (3.2). Thus, we obtain following relations:

$$h_1 = \delta h^e h_1^*$$  \hfill (3.18)
$$h_2 = \delta h^e h_2^*$$  \hfill (3.19)

Note that the characteristic pressure drop $\delta h^e$ is the same for both sub-domains, since it results from the macroscopic boundary and initial conditions. We also introduce the dimensionless time variable $t^*$ and two dimensionless spatial variables $x$ and $y$:

$$t^* = t/T$$  \hfill (3.20)
$$x = X/L$$  \hfill (3.21)
$$y = X/l$$  \hfill (3.22)

where $T$ is the characteristic time, $x$ is the dimensionless macroscopic variable and $y$ is the dimensionless local variable. Introducing the relations (3.18)–(3.22) into (3.10)–(3.11) leads to the following dimensionless equations:

$$\frac{\partial^2 C_1^c}{T K_1^c} \frac{\partial h_1^*}{\partial t^*} - \frac{\partial}{\partial y_i} \left[ K_{1ij}^* \frac{\partial}{\partial y_j} \left( h_1^* + \frac{l}{\delta h^e} y_3 \right) \right] = 0 \quad \text{in } \Omega_1$$  \hfill (3.23)
$$\frac{\partial^2 C_2^c}{T K_2^c} \frac{\partial h_2^*}{\partial t^*} - \frac{\partial}{\partial y_i} \left[ K_{2ij}^* \frac{\partial}{\partial y_j} \left( h_2^* + \frac{l}{\delta h^e} y_3 \right) \right] = 0 \quad \text{in } \Omega_2$$  \hfill (3.24)

with the conditions on $\Gamma$:

$$\delta h^e h_1^* = \delta h^e h_2^*$$ \quad \text{on } $\Gamma$  \hfill (3.25)

$$\left[ K_{1i}^* \frac{\partial}{\partial y_i} \left( h_1^* + \frac{l}{\delta h^e} y_3 \right) \right] N_i = \left[ K_{2i}^* \frac{\partial}{\partial y_i} \left( h_2^* + \frac{l}{\delta h^e} y_3 \right) \right] N_i \quad \text{on } \Gamma \hfill (3.26)$$

The equations (3.23)–(3.26) are normalized with respect to the size of the period $l$. As we can see, three dimensionless parameters appear in (3.23)–(3.24), namely $\frac{C_1^c}{TK_1^c}$, $\frac{l}{\delta h^e}$ and $\frac{K_2^c}{K_1^c}$. They characterize the regime of the flow. Before proceeding with the homogenization procedure one has to estimate the order of magnitude of this parameters. The estimations are made with regard to the scale parameter $\varepsilon$. In this way the dimensionless numbers are replaced by different powers of $\varepsilon$.

The asymptotic expansions (3.5) are introduced into the normalized equations (3.23)–(3.26) and the two-scale derivation operator (3.8) is applied. This leads to a series of differential problems corresponding to different powers of $\varepsilon$. The problems are successively solved over the period domain $\Omega$. This procedure will be applied to derive the macroscopic models for two particular cases of the local geometry — soil with weakly conductive inclusions (Section 3.3) and soil with highly conductive inclusions (Section 3.4).
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3.3 Soil with weakly conductive inclusions

(Lewandowska et al., 2004b)

3.3.1 Parameter estimation and dimensionless problem

In this section we consider a typical double-porosity medium consisting of weakly conductive inclusions embedded in a highly conductive matrix — Fig. 3.1. The chosen observation time $T$ corresponds to the time of flow in the more conductive region at the macroscopic scale, which implies the following relation:

$$T = \frac{C_c^1 L^2}{K_c^1} = \frac{L^2}{D_c^c}$$  \hspace{1cm} (3.27)

We assume the characteristic diffusivity of the two sub-domains satisfies the following relation:

$$\frac{D_c^2}{D_c^1} = \frac{K_c^2}{C_c^2} \frac{C_c^1}{K_c^1} = O(\varepsilon^2)$$  \hspace{1cm} (3.28)

Taking into account the definition of $\varepsilon$ (3.1) we obtain:

$$T = \frac{C_c^1 L^2}{K_c^1} = \frac{l^2}{D_c^2}$$  \hspace{1cm} (3.29)

The diffusivity is expressed by the capillary capacity and the hydraulic conductivity. Thus, the estimation (3.27) holds for different combination of $K_c^2/K_c^1$ and $C_c^1/C_c^2$ ratio. In this section we assume that the characteristic capillary capacity is of the same order in the two sub-domains. The contrast in transfer properties comes from the hydraulic conductivity ratio:

$$\frac{C_c^1}{C_c^2} = O(1) \hspace{1cm} \frac{K_c^2}{K_c^1} = O(\varepsilon^2)$$  \hspace{1cm} (3.30)

The case of different $C_c^1/C_c^2$ ratio is discussed at the end of this chapter.

At the scale of a single period, the capillary effects are dominating over the gravity effects:

$$\frac{l}{\delta h^c} = O(\varepsilon)$$  \hspace{1cm} (3.31)

In other words, we assume that the gravitational potential gradient is much smaller locally than the pressure potential gradient. This assumption holds when the size of inclusions is not very large and it is justified in many practical applications concerning aggregated soils. The situation could be different when the inclusions had a form of very large porous blocks, as it is encountered in fractured reservoir simulations. Such case was studied by Arbogast (1993a,b). Note that our hypotheses refers only to the local conditions and does not remove gravity from the macroscopic model.
Introducing the estimations (3.27)–(3.31) into the normalized equations (3.23)–(3.26) one obtains:

\[
\varepsilon^2 C_1^* \frac{\partial h_1^*}{\partial \ell^*} - \frac{\partial}{\partial y_i} \left[ K_{1ij}^* \frac{\partial}{\partial y_j} \left( h_1^* + \varepsilon y_3 \right) \right] = 0 \quad \text{in } \Omega_1 (3.32)
\]

\[
C_2^* \frac{\partial h_2^*}{\partial \ell^*} - \frac{\partial}{\partial y_i} \left[ K_{2ij}^* \frac{\partial}{\partial y_j} \left( h_2^* + \varepsilon y_3 \right) \right] = 0 \quad \text{in } \Omega_2 (3.33)
\]

with the interface conditions:

\[
h_1^* = h_2^* \quad \text{on } \Gamma (3.34)
\]

\[
\left[ K_{1ij}^* \frac{\partial}{\partial y_j} \left( h_1^* + y_3 \right) \right] N_i = \varepsilon^2 \left[ K_{2ij}^* \frac{\partial}{\partial y_j} \left( h_2^* + y_3 \right) \right] N_i \quad \text{on } \Gamma (3.35)
\]

Note that all terms in (3.32)–(3.35) are of the order \( \mathcal{O}(1) \). The factor \( \varepsilon^2 \) in (3.32) and (3.35) comes from the contrast between the hydraulic properties of the two sub-domains.

### 3.3.2 Macroscopic variable

Let us analyze the behavior of the water pressure head at the first order of approximation.

From (3.32) and (3.35) we extract problems corresponding to the power \( \varepsilon^0 \) as follows:

\[
\frac{\partial}{\partial y_i} \left[ K_{1ij}^{(0)} \frac{\partial h_1^{(0)}}{\partial y_j} \right] = 0 \quad i, j = 1, 2, 3 \quad \text{in } \Omega_1 (3.36)
\]

\[
\left[ K_{1ij}^{(0)} \frac{\partial h_1^{(0)}}{\partial y_j} \right] N_i = 0 \quad \text{on } \Gamma (3.37)
\]

where \( h_1^{(0)} \) is \( y \)-periodic. It can be shown that the solution of the nonlinear problem (3.36)–(3.37) is a function which depends on the macroscopic space variable \( x \) and does not depend on the local space variable \( y \) (Auriault & Lewandowska, 1997; Bensoussan et al., 1978; Sanchez-Palencia, 1980):

\[
h_1^{(0)} = h_1^{(0)}(x, \ell^*) (3.38)
\]

To prove this result let us multiply (3.36) by \( h_1^{(0)} \) and integrate over \( \Omega_1 \):

\[
\int_{\Omega_1} h_1^{(0)} \frac{\partial}{\partial y_i} \left[ K_{1ij}^{(0)} \frac{\partial h_1^{(0)}}{\partial y_j} \right] \, d\Omega = 0 (3.39)
\]

Then, the following transformations are possible:

\[
\int_{\Omega_1} \frac{\partial}{\partial y_i} \left[ h_1^{(0)} K_{1ij}^{(0)} \frac{\partial h_1^{(0)}}{\partial y_j} \right] \, d\Omega - \int_{\Omega_1} K_{1ij}^{(0)} \frac{\partial h_1^{(0)}}{\partial y_i} \frac{\partial h_1^{(0)}}{\partial y_j} \, d\Omega = 0 (3.40)
\]

\[
\int_{S_1} h_1^{(0)} K_{1ij}^{(0)} \frac{\partial h_1^{(0)}}{\partial y_j} N_i \, dS_1 - \int_{\Omega_1} K_{1ij}^{(0)} \frac{\partial h_1^{(0)}}{\partial y_i} \frac{\partial h_1^{(0)}}{\partial y_j} \, d\Omega = 0 (3.41)
\]
In the above transformations we applied first the integration by parts and then the divergence theorem to pass from volume integral over \( \Omega_1 \) to the surface integral over its boundary \( S_1 \). Note that \( S_1 \) is the sum of outer boundary of the period \( \partial \Omega \) and the interface \( \Gamma \). Due to the periodicity the integral over \( \partial \Omega \) disappears. Moreover, from (3.37) result that the integral over interface is equal to zero. Since the whole expression should yield zero (due to (3.36)), the second term in the expression (3.41) must also vanish.

\[
\int_{\Omega_1} K^{(0)}_{ij} \frac{\partial h^{(0)}_1}{\partial y_i} \frac{\partial h^{(0)}_1}{\partial y_j} \, d\Omega = 0 \quad (3.42)
\]

where \( K^{(0)}_{ij} = K_{ij}(h^{(0)}_1) > 0 \). Consequently, the gradients of \( h^{(0)}_1 \) with respect to \( y_i \) must be equal to zero, which means that \( h^{(0)}_1 \) is independent of \( y \).

Thus, the first order solution \( h^{(0)}_1 \) is constant over the period and it can be concluded that \( h^{(0)}_1 \) is a macroscopic variable, which will be denoted \( h^{(0)} \). From the water retention curve we also obtain the corresponding water content in \( \Omega_1 \), \( \theta^{(0)}_1 = \theta_1(h^{(0)}_1) \).

### 3.3.3 Local boundary value problem

The local boundary value problem follows from (3.32) and (3.35) at the power of \( \varepsilon^1 \):

\[
\frac{\partial}{\partial y_i} \left[ K^{(0)}_{ij} \left( \frac{\partial h^{(0)}_1}{\partial x_j} + I_j \right) + K^{(0)}_{ij} \frac{\partial h^{(1)}_1}{\partial y_j} \right] = 0 \quad i, j = 1, 2, 3 \quad \text{in } \Omega_1 \quad (3.43)
\]

\[
\left[ K^{(0)}_{ij} \left( \frac{\partial h^{(0)}_1}{\partial x_j} + I_j \right) + K^{(0)}_{ij} \frac{\partial h^{(1)}_1}{\partial y_j} \right] N_i = 0 \quad \text{on } \Gamma \quad (3.44)
\]

where the term \( I_j \) is a component of the identity matrix \( I \) representing the gravity and \( h^{(0)}_1 \) is \( y \)-periodic. It can be shown (Auriault & Lewandowska, 1997; Bensoussan et al., 1978; Sanchez-Palencia, 1980) that the solution of (3.43)–(3.44) has the form of a linear function of the macroscopic gradient \( \left( \frac{\partial h^{(0)}_1}{\partial x_i} + I_3 \right) \):

\[
h^{(1)}_1 = \chi_i \left( \frac{\partial h^{(0)}_1}{\partial x_i} + I_3 \right) + \tilde{h}^{(1)}(x, t^*) \quad (3.45)
\]

where \( \tilde{h}^{(1)} \) is an arbitrary function of \( x \) and \( t^* \) and \( \chi \) is a vector function of the local variable \( y \). Introduction of (3.45) into the problem (3.43)–(3.44) yields:

\[
\frac{\partial}{\partial y_i} \left[ K^{(0)}_{ij} \left( \frac{\partial h^{(0)}_1}{\partial x_j} + I_j \right) + K^{(0)}_{ij} \frac{\partial}{\partial y_j} \left[ \chi_k \left( \frac{\partial h^{(0)}_1}{\partial x_k} + I_3 \right) + \tilde{h}^{(1)} \right] \right] = 0 \quad (3.46)
\]

\[
\left[ K^{(0)}_{ij} \left( \frac{\partial h^{(0)}_1}{\partial x_j} + I_j \right) + K^{(0)}_{ij} \frac{\partial}{\partial y_j} \left[ \chi_k \left( \frac{\partial h^{(0)}_1}{\partial x_k} + I_3 \right) + \tilde{h}^{(1)} \right] \right] N_i = 0 \quad (3.47)
\]
The function $\bar{h}^{(1)}$ is independent of $y$, thus one obtains:

$$\frac{\partial}{\partial y_i} \left[ K_{1ij}^{(0)} \left( \frac{\partial h^{(0)}}{\partial x_j} + I_{j3} \right) + K_{1ij}^{(0)} \frac{\partial}{\partial y_j} \left[ \chi_k \left( \frac{\partial h^{(0)}}{\partial x_k} + I_{k3} \right) \right] \right] = 0 \quad (3.48)$$

In order to calculate the values of $\chi$, let us impose a unit macroscopic gradient $\left( \frac{\partial h^{(0)}}{\partial x_i} + I_{i3} \right) = 1$. The problem (3.48)–(3.49) becomes:

$$\frac{\partial}{\partial y_i} \left[ K_{1ij}^{(0)} \left( I_{jk} + \frac{\partial \chi_k}{\partial y_j} \right) \right] = 0 \quad i, j, k = 1, 2, 3 \quad \text{in } \Omega_1 \quad (3.50)$$

$$\left[ K_{1ij}^{(0)} \left( I_{jk} + \frac{\partial \chi_k}{\partial y_j} \right) \right] N_i = 0 \quad \text{on } \Gamma \quad (3.51)$$

The vector function $\chi$ has zero-valued volume average:

$$\langle \chi \rangle = \frac{1}{|\Omega|} \int_{\Omega} \chi \, d\Omega = 0 \quad (3.52)$$

Moreover, $\chi$ is $y$-periodic. Each component of the vector $\chi$ ($\chi_1, \chi_2, \chi_3$) is a function of three space coordinates ($y_1, y_2, y_3$). The function $\chi$ characterizes the influence of the local geometry of the period on macroscopic transfer properties. The solution of the problem (3.50)–(3.52) requires information on the period geometry. Except for some particular cases, the problem has to be solved numerically.

When the local conductivity $K_1$ is isotropic and constant over the $\Omega_1$ sub-domain, the local boundary value problem (3.50)–(3.51) can be written in the following form:

$$\frac{\partial}{\partial y_i} \left[ I_{ik} + \frac{\partial \chi_k}{\partial y_i} \right] = 0 \quad i, k = 1, 2, 3 \quad \text{in } \Omega_1 \quad (3.53)$$

$$\left[ I_{ik} + \frac{\partial \chi_k}{\partial y_i} \right] N_i = 0 \quad \text{on } \Gamma \quad (3.54)$$

### 3.3.4 Local flow in inclusions

From equations (3.33) and (3.34) at the order $\varepsilon^0$ one obtains a nonlinear boundary value problem for the water pressure head in the sub-domain $\Omega_2$.

$$C_{2}^{(0)} \frac{\partial h_2^{(0)}}{\partial t} + \frac{\partial}{\partial y_i} \left( K_{2ij}^{(0)} \frac{\partial h_2^{(0)}}{\partial y_j} \right) = 0 \quad \text{in } \Omega_2 \quad (3.55)$$

$$h_2^{(0)} = h^{(0)} \quad \text{on } \Gamma \quad (3.56)$$

Since $h_2^{(0)}$ is not constant over the sub-domain $\Omega_2$, it is not a macroscopic variable. It can be concluded that local non-equilibrium conditions arise during the flow process. We have
two water pressure head fields — macroscopic \( h^{(0)} \) and local \( h_2^{(0)} \) which are coupled by the boundary condition (3.56). The interaction is complex due to the nonlinearity of the problem (3.55)–(3.56). Note also that gravity does not influence the local flow, which results from the assumption (3.31).

### 3.3.5 Macroscopic flow equation

In order to determine the macroscopic model let us write equations (3.32) and (3.35) at the order \( \varepsilon^2 \):

\[
C_1^{(0)} \frac{\partial h^{(0)}}{\partial t^*} - \frac{\partial}{\partial y_i} \left[ K_{1ij}^{(0)} \left( \frac{\partial h_1^{(1)}}{\partial x_j} + \frac{\partial h_1^{(2)}}{\partial y_j} \right) + K_{1ij}^{(1)} \left( \frac{\partial h_0^{(0)}}{\partial x_j} + \frac{\partial h_1^{(1)}}{\partial y_j} \right) \right] + K_{1ij}^{(1)} \left( \frac{\partial h_0^{(0)}}{\partial x_j} + \frac{\partial h_1^{(1)}}{\partial y_j} \right) + K_{1ij}^{(1)} I_j = 0 \quad (3.57)
\]

\[
\left[ K_{1ij}^{(0)} \left( \frac{\partial h_1^{(1)}}{\partial x_j} + \frac{\partial h_1^{(2)}}{\partial y_j} \right) + K_{1ij}^{(1)} \left( \frac{\partial h_0^{(0)}}{\partial x_j} + \frac{\partial h_1^{(1)}}{\partial y_j} \right) + K_{1ij}^{(1)} I_j \right] N_i = K_{2ij}^{(0)} \frac{\partial h_{2ij}^{(0)}}{\partial y_j} \quad (3.58)
\]

Let us integrate equation (3.57) over \( \Omega_1 \) and divide it by \(|\Omega|\):

\[
\frac{1}{|\Omega|} \int_{\Omega_1} \left\{ C_1^{(0)} \frac{\partial h^{(0)}}{\partial t^*} + \frac{\partial}{\partial y_i} \left[ K_{1ij}^{(0)} \left( \frac{\partial h_1^{(1)}}{\partial x_j} + \frac{\partial h_1^{(2)}}{\partial y_j} \right) + K_{1ij}^{(1)} \left( \frac{\partial h_0^{(0)}}{\partial x_j} + \frac{\partial h_1^{(1)}}{\partial y_j} \right) + K_{1ij}^{(1)} I_j \right] + K_{1ij}^{(1)} \left( \frac{\partial h_0^{(0)}}{\partial x_j} + \frac{\partial h_1^{(1)}}{\partial y_j} \right) + K_{1ij}^{(1)} I_j \right\} d\Omega = 0 \quad (3.59)
\]

The next four steps concern transformation of the second term of (3.59). First we apply the Gauss-Ostrogradski theorem to the second term to transform the volume integral to the surface integral:

\[
-\frac{1}{|\Omega|} \int_{\Omega_1} \frac{\partial}{\partial y_i} \left[ K_{1ij}^{(0)} \left( \frac{\partial h_1^{(1)}}{\partial x_j} + \frac{\partial h_1^{(2)}}{\partial y_j} \right) + K_{1ij}^{(1)} \left( \frac{\partial h_0^{(0)}}{\partial x_j} + \frac{\partial h_1^{(1)}}{\partial y_j} \right) + K_{1ij}^{(1)} I_j \right] d\Omega = \frac{1}{|\Omega|} \int_{\partial \Omega_1} \left[ K_{1ij}^{(0)} \left( \frac{\partial h_1^{(1)}}{\partial x_j} + \frac{\partial h_1^{(2)}}{\partial y_j} \right) + K_{1ij}^{(1)} \left( \frac{\partial h_0^{(0)}}{\partial x_j} + \frac{\partial h_1^{(1)}}{\partial y_j} \right) + K_{1ij}^{(1)} I_j \right] N_i dS_i \quad (3.60)
\]
where $S_1$ is the boundary of $\Omega_1$. It is a sum of the outer boundary of the period $\partial \Omega$ and the interface $\Gamma$. Due to the periodicity conditions the integral over $\partial \Omega$ is equal to zero. The integration over $\Gamma$ using (3.58) yields:

$$\frac{1}{|\Omega|} \int_{\Gamma} \left[ K_{1ij}^{(0)} \left( \frac{\partial h_1^{(1)}}{\partial x_j} + \frac{\partial h_1^{(2)}}{\partial y_j} \right) + K_{1ij}^{(1)} \left( \frac{\partial h_0^{(0)}}{\partial x_j} + \frac{\partial h_1^{(1)}}{\partial y_j} \right) + K_{1ij}^{(1)} I_{3j} \right] N_i \, d\Gamma =$$

$$= \frac{1}{|\Omega|} \int_{\Gamma} \left[ K_{2ij}^{(0)} \frac{\partial h_2^{(0)}}{\partial y_j} \right] N_i \, d\Gamma \quad (3.61)$$

We apply once again the Gauss-Ostrogradski theorem to pass from the surface to the volume integral over $\Omega_2$ and we make use of the equation (3.55):

$$\frac{1}{|\Omega|} \int_{\Gamma} \left[ K_{2ij}^{(0)} \frac{\partial h_2^{(0)}}{\partial y_j} \right] N_i \, d\Gamma = \frac{1}{|\Omega|} \int_{\Omega_2} C_{2}^{(0)} \frac{\partial h_2^{(0)}}{\partial t^*} \, d\Omega \quad (3.62)$$

Finally, we use the solution (3.45) for $h_1^{(1)}$ in the third term of (3.59). After these transformations one obtains the macroscopic model in the following form:

$$C^{\text{eff}} \frac{\partial h_0^{(0)}}{\partial t^*} - \frac{\partial}{\partial x_i} \left[ K^{\text{eff}} \frac{\partial}{\partial x_j} \left( h_0^{(0)} + x_3 \right) \right] + \frac{1}{|\Omega|} \int_{\Omega_2} C_{2}^{(0)} \frac{\partial h_2^{(0)}}{\partial t^*} = 0 \quad (3.63)$$

The macroscopic model has the form of a single highly nonlinear integro-differential equation. Both capillary and gravity forces are present at the macroscopic scale. The flow is governed by two effective parameters — $C^{\text{eff}}$ and $K^{\text{eff}}$. The effective capillary capacity is defined as:

$$C^{\text{eff}}(h_0^{(0)}) = \frac{1}{|\Omega|} \int_{\Omega_1} C_1^{(0)} \, d\Omega = w_1 C_1^{(0)} \quad (3.64)$$

where $C_1^{(0)} = C_1(h_0^{(0)})$. The retention term in (3.63) can be also written as:

$$C^{\text{eff}} \frac{\partial h_0^{(0)}}{\partial t^*} = \frac{\partial \theta^{av}}{\partial t} \quad (3.65)$$

where $\theta^{av}$ is the volumetric water content in sub-domain $\Omega_1$, averaged with respect to the total volume of the period. Note that the total water content in the period is calculated as:

$$\theta^{tot} = \theta^{av} + \frac{1}{|\Omega|} \int_{\Omega_2} \theta_2 \, d\Omega \quad (3.66)$$

The definition of the effective conductivity tensor results from substituting (3.45) into (3.59):

$$K_i^{\text{eff}}(h_0^{(0)}) = \frac{1}{|\Omega|} \int_{\Omega_1} K_{1ik}^{(0)} \left( I_{kj} + \frac{\partial \chi_j}{\partial y_k} \right) \, d\Omega_1 \quad (3.67)$$

where the function $\chi$ is the solution of the local boundary value problem (3.50)–(3.51). It can be shown that $K$ is symmetric and positively definite (Auriault & Lewandowska, 1997).
If the local conductivity tensor $K_1$ is isotropic and constant over $\Omega_1$ the definition (3.67) becomes:

$$K^{\text{eff}}_{ij}(h^{(0)}) = \frac{K_1}{|\Omega_1|} \int_{\Omega_1} \left(I_{ij} + \frac{\partial \chi_j}{\partial y_i}\right) d\Omega_1 \quad (3.68)$$

with $K_1^{(0)} = K_1(h^{(0)})$. Note that both effective parameters depend on the local characteristics of the more conductive sub-domain and on the local geometry. They are independent of the parameters of the weakly conductive inclusions.

The integral source term in (3.63) describes the local non-equilibrium effects. It represents the rate of change of the average water content in the inclusions:

$$\frac{1}{|\Omega_2|} \int_{\Omega_2} C_2^{(0)} \frac{\partial h_2^{(0)}}{\partial t^*} d\Omega = \frac{1}{|\Omega_2|} \int_{\Omega_2} \frac{\partial \theta_2^{(0)}}{\partial t^*} d\Omega \quad (3.69)$$

The water pressure head $h_2^{(0)}$ and the water content $\theta_2(h_2^{(0)})$ are locally variable in the period. Their distribution is obtained from the solution of the equation (3.55) with the coupling boundary condition (3.56). Thus, the model (3.63) has complex structure. At each point of the macroscopic domain $x$ one has to solve an additional equation in local coordinates $y$ describing the flow in inclusions. The numerical implementation of this model is presented in Chapter 4.

Note also that the presence of double-porosity (non-equilibrium) effects is closely related to the choice of the observation time. Other estimations of the parameters are also possible, which will be discussed in Section 3.5.

### 3.3.6 Discussion

The model (3.63) consists of a single highly nonlinear integro-differential equation with two effective parameters. The effective capacity and effective conductivity depend on the characteristics of the more conductive interconnected sub-domain. They are independent of the hydraulic parameters of the weakly conductive sub-domain. The influence of the less conductive regions is taken into account by the source term in the macroscopic equation. The calculation of that integral requires a local-scale flow equation to be solved at each point of the macroscopic domain. Similar models were obtained by other authors using asymptotic homogenization to describe flow in double-porosity media. (Hornung, 1991; Arbogast et al., 1990; Arbogast, 1993a,b).

The comparison of the structure of the model obtained by homogenization with other double-porosity models existing in literature reveals several important points. Homogenization leads to a one-equation model, like the dual-porosity model of Zimmerman et al. (1996), where the inclusions act only as source term. The presented model is different from
the dual-permeability models proposed for example by Barenblatt et al. (1960), Gerke & van Genuchten (1993a) or Quintard & Whitaker (1996). In those models two macroscopic pressure fields appear. In the model (3.63) the pressure head in less conductive sub-domain remains a local variable. As it was pointed out by Quintard & Whitaker (1996), the two-equation approach is suitable for quasi-steady flow, whereas for highly transient flow the macroscopization procedure leads to models with coupled local and macroscopic variables, similar to the one presented here.

One should note that the analysis presented in this section remains valid if the less conductive regions are interconnected. The flow can be described by the same macroscopic equation (3.63) as long as the parameter estimations (3.27)–(3.31) hold. If the diffusivity ratio is small enough \( \frac{D_2}{D_1} = \mathcal{O}(\varepsilon^2) \) and the separation of scales is satisfied, the flow in less conductive regions is caused mainly by the water transfer from the more conductive sub-domain.

Another important issue is the estimation of the water exchange rate between the two sub-domains. In the phenomenological double-porosity models this interaction is usually described by some simple analytical formulas (Zimmerman et al., 1996; Gerke & van Genuchten, 1993b, 1996) Application of analytical approximations of the exchange term reduces significantly the computational time, usually at the cost of accuracy. Such simplifications may be necessary from the point of view of practical applications. Using the presented model obtained by homogenization the simplifications can be done in a controlled and rigorous way. Note that Quintard & Whitaker (1996) developed a mathematically rigorous procedure for the estimation of the transfer coefficients when the quasi-steady first order approximation for the exchange term holds. However, their study concerned the case of slightly compressible single-phase flow, which is described by linear equations.

Finally, the up-scaling methods (either homogenization or volume averaging) allow to estimate accurately the effective parameters of the medium, provided that the local characteristics of the two regions and geometry are known. In contrast, the phenomenological double-porosity models often provide only little guidance on the estimation of the effective parameters. For example in the model of Gerke & van Genuchten (1993a) the effective conductivities of the two sub-domains are equal to \( w_1K_1 \) and \( w_2K_2 \), where \( w_1 \) and \( w_2 \) are the volumetric fractions of each component. Such estimation is true only for a particular geometry, when the medium is layered and the flow is parallel to the layers. We show that in general the effective conductivity depends not only on the volumetric fraction but also on the geometry of inclusions. For simple forms of inclusions (spheres, cubes) the effective conductivity can be calculated as function of \( w_1 \), but it is less than \( w_1K_1 \) (see Chapter 5).
3.4 Soil with highly conductive inclusions

(Lewandowska & Auriault, 2004), (Lewandowska et al., 2004a)

3.4.1 Parameter estimation and dimensionless problem

In this section we analyze the macroscopic behavior of soil with highly conductive inclusions. It means that the more conductive sub-domain $\Omega_1$ is not interconnected and the process is governed by the less conductive matrix $\Omega_2$. Thus, we choose the time of flow in matrix at the macroscopic scale as the characteristic observation time $T$:

$$T = \frac{C^*_c L^2}{K^*_2} = \frac{L^2}{D^*_2}$$  \hspace{1cm} (3.70)

We assume that the diffusivity ratio is:

$$\frac{D^*_2}{D^*_1} = \mathcal{O}(\varepsilon)$$  \hspace{1cm} (3.71)

which corresponds to the following relations of the capillary capacity and the hydraulic conductivity:

$$\frac{K^*_2}{K^*_1} = \mathcal{O}(\varepsilon), \quad \frac{C^*_2}{C^*_1} = \mathcal{O}(1)$$  \hspace{1cm} (3.72)

As in the previous case, we assume that at the local scale the gravity effects are small compared to the capillary effects (3.31). These estimations lead to the following normalized equations:

$$\varepsilon^3 C^*_1 \frac{\partial h^*_1}{\partial t^*} - \frac{\partial}{\partial y_i} \left[ K^*_1 \frac{\partial}{\partial y_i} (h^*_1 + \varepsilon y_3) \right] = 0 \quad i, j = 1, 2, 3 \quad \text{in } \Omega_1$$  \hspace{1cm} (3.73)

$$\varepsilon^2 C^*_2 \frac{\partial h^*_2}{\partial t^*} - \frac{\partial}{\partial y_i} \left[ K^*_2 \frac{\partial}{\partial y_i} (h^*_2 + \varepsilon y_3) \right] = 0 \quad \text{in } \Omega_2$$  \hspace{1cm} (3.74)

with the conditions at the interface:

$$h^*_1 = h^*_2$$  \hspace{1cm} on $\Gamma$  \hspace{1cm} (3.75)

$$\left[ K^*_1 \frac{\partial}{\partial y_j} (h^*_1 + \varepsilon y_3) \right] N_i = \varepsilon \left[ K^*_2 \frac{\partial}{\partial y_j} (h^*_2 + \varepsilon y_3) \right] N_i \quad \text{on } \Gamma$$  \hspace{1cm} (3.76)

In the following part we apply the same homogenization technique as described in the previous section, i.e. the asymptotic expansions and the two-scale operator are introduced into (3.73)–(3.76). The macroscopic model will be found by solving the problems appearing at successive orders of $\varepsilon$. 

65
3.4.2 Macroscopic variable

Let us write equations (3.73)–(3.76) at the power $\varepsilon^0$:

\[
\frac{\partial}{\partial y_i} \left[ K_{ij}^{(0)} \frac{\partial h_{1}^{(0)}}{\partial y_j} \right] = 0 \quad \text{in} \; \Omega_1 \tag{3.77}
\]

\[
\frac{\partial}{\partial y_i} \left[ K_{ij}^{(0)} \frac{\partial h_{2}^{(0)}}{\partial y_j} \right] = 0 \quad \text{in} \; \Omega_2 \tag{3.78}
\]

and:

\[
h_{1}^{(0)} = h_{2}^{(0)} \quad \text{on} \; \Gamma \tag{3.79}
\]

\[
\left[ K_{ij}^{(0)} \frac{\partial h_{1}^{(0)}}{\partial y_j} \right] N_i = 0 \quad \text{on} \; \Gamma \tag{3.80}
\]

where $h_{2}^{(0)}$ is $y$-periodic. It can be shown (Bensoussan et al., 1978; Sanchez-Palencia, 1980) that the solution of the problem (3.77)–(3.80) is independent of the local space variable $y$:

\[
h_{1}^{(0)} = h_{2}^{(0)} = h^{(0)}(x, t^*) \tag{3.81}
\]

This result can be proved in a similar manner as presented in section 3.3.2. First, let us note that (3.77) and (3.80) constitute a problem equivalent to (3.36)–(3.37). Thus one obtains $h_{1}^{(0)} = h_{1}^{(0)}(x, t^*)$. Then, we apply analogous procedure to (3.78). Multiplying the equation by $h_{2}^{(0)}$, integrating by parts and taking into account the periodicity and boundary conditions we obtain $h_{2}^{(0)} = h_{2}^{(0)}(x, t^*) = h_{1}^{(0)}(x, t^*)$. It means that we have only one water pressure head field and the equilibrium conditions exist at the first order of approximation.

3.4.3 Local boundary value problem

Taking into account the result (3.81) the following problems arise at the power $\varepsilon^1$:

\[
\frac{\partial}{\partial y_i} \left[ K_{1ij}^{(0)} \left( \frac{\partial h_{1}^{(0)}}{\partial x_j} + I_{j3} \right) + K_{1ij}^{(0)} \frac{\partial h_{1}^{(1)}}{\partial y_j} \right] = 0 \quad \text{in} \; \Omega_1 \tag{3.82}
\]

\[
\frac{\partial}{\partial y_i} \left[ K_{2ij}^{(0)} \left( \frac{\partial h_{2}^{(0)}}{\partial x_j} + I_{j3} \right) + K_{2ij}^{(0)} \frac{\partial h_{2}^{(1)}}{\partial y_j} \right] = 0 \quad \text{in} \; \Omega_2 \tag{3.83}
\]

and:

\[
h_{1}^{(1)} = h_{2}^{(1)} \quad \text{on} \; \Gamma \tag{3.84}
\]

\[
\left[ K_{1ij}^{(0)} \left( \frac{\partial h_{1}^{(0)}}{\partial x_j} + I_{j3} \right) + K_{1ij}^{(0)} \frac{\partial h_{1}^{(1)}}{\partial y_j} \right] N_i = 0 \quad \text{on} \; \Gamma \tag{3.85}
\]
where $h_2^{(1)}$ is y-periodic. In order to solve this problem let us multiply (3.82) by 
\[ -y_i \left( \frac{\partial h_0^{(0)}}{\partial x_i} + I_{i3} \right) + h_1^{(1)} \] and integrate it over $\Omega_1$:

\[
\int_{\Omega_1} \left[ -y_i \left( \frac{\partial h_0^{(0)}}{\partial x_i} + I_{i3} \right) + h_1^{(1)} \right] \frac{\partial}{\partial y_i} \left[ K_{1ij}^{(0)} \left( \frac{\partial h_0^{(0)}}{\partial x_j} + I_{j3} \right) + K_{1ij}^{(0)} \frac{\partial h_1^{(1)}}{\partial y_j} \right] \, d\Omega = 0 \tag{3.86}
\]

After some transformations we obtain the following equation:

\[
\int_{\Omega_1} \left[ \left( \frac{\partial h_0^{(0)}}{\partial x_i} + I_{i3} \right) + \frac{\partial h_1^{(1)}}{\partial y_i} \right] \left[ K_{1ij}^{(0)} \left( \frac{\partial h_0^{(0)}}{\partial x_j} + I_{j3} \right) + K_{1ij}^{(0)} \frac{\partial h_1^{(1)}}{\partial y_j} \right] \, d\Omega = 0 \tag{3.87}
\]

Taking into account the positivity of the tensor $K$, equation (3.87) implies that:

\[
\left[ \left( \frac{\partial h_0^{(0)}}{\partial x_i} + I_{i3} \right) + \frac{\partial h_1^{(1)}}{\partial y_i} \right] = 0 \tag{3.88}
\]

Therefore, the solution of the problem (3.82) and (3.85) can be put in the form:

\[
h_1^{(1)} = -y_i \left( \frac{\partial h_0^{(0)}}{\partial x_i} + I_{i3} \right) + \bar{h}_1^{(1)}(x, t^*) \tag{3.89}
\]

Consequently, the problem (3.83) and (3.84) yields:

\[
h_1^{(1)} = \chi_i \left( \frac{\partial h_0^{(0)}}{\partial x_i} + I_{i3} \right) + \bar{h}_2^{(1)}(x, t^*) \tag{3.90}
\]

with:

\[
\bar{h}_1^{(1)}(x, t^*) = \bar{h}_2^{(1)}(x, t^*) = \bar{h}^{(1)}(x, t^*) \tag{3.91}
\]

where $\bar{h}^{(1)}$ is an arbitrary scalar function of $x$ and $t^*$. The vector function $\chi$ is obtained by substituting (3.90) into (3.83) and (3.84), which yields the following local boundary value problem:

\[
\frac{\partial}{\partial y_i} \left[ K_{2ij}^{(0)} \left( I_{jk} - \frac{\partial \chi_k}{\partial y_j} \right) \right] = 0 \quad i, j, k = 1, 2, 3 \quad \text{in } \Omega_2 \quad \chi_k = y_k \quad \text{on } \Gamma \tag{3.92}
\]

\[
\chi_k = y_k \quad \text{on } \Gamma \tag{3.93}
\]

and $\chi$ is y–periodic. Solution of this problem requires information on the local geometry of the period. If the local conductivity is isotropic and constant in $\Omega_2$ the problem (3.92) – (3.93) becomes:

\[
\frac{\partial}{\partial y_i} \left[ I_{ik} - \frac{\partial \chi_k}{\partial y_i} \right] = 0 \quad i, k = 1, 2, 3 \quad \text{in } \Omega_2 \tag{3.94}
\]

\[
\chi_k = y_k \quad \text{on } \Gamma \tag{3.95}
\]
3.4.4 Macroscopic flow equation

In order to determine the macroscopic model let us write the corresponding problems in both sub-domains. Equation (3.73) at the order $\varepsilon^3$ gives:

\[
C_1^{(0)} \frac{\partial h^{(0)}}{\partial t^*} - \frac{\partial}{\partial y_i} \left[ K_{1ij}^{(0)} \left( \frac{\partial h_i^{(2)}}{\partial x_j} + \frac{\partial h_i^{(3)}}{\partial y_j} \right) + K_{1ij}^{(1)} \left( \frac{\partial h_i^{(1)}}{\partial x_j} + \frac{\partial h_i^{(2)}}{\partial y_j} \right) + \right. \\
+ K_{1ij}^{(2)} \left( \frac{\partial h_i^{(0)}}{\partial x_j} + \frac{\partial h_i^{(1)}}{\partial y_j} \right) + K_{1ij}^{(2)} I_{3j} \left] + \\
- \frac{\partial}{\partial x_i} \left[ K_{1ij}^{(0)} \left( \frac{\partial h_i^{(1)}}{\partial x_j} + \frac{\partial h_i^{(2)}}{\partial y_j} \right) + K_{1ij}^{(1)} \left( \frac{\partial h_i^{(0)}}{\partial x_j} + \frac{\partial h_i^{(1)}}{\partial y_j} \right) + K_{1ij}^{(1)} I_{3j} \right] = 0 \quad (3.96)
\]

Equation (3.74) at the order $\varepsilon^2$ gives:

\[
C_2^{(0)} \frac{\partial h^{(0)}}{\partial t^*} - \frac{\partial}{\partial y_i} \left[ K_{2ij}^{(0)} \left( \frac{\partial h_i^{(2)}}{\partial x_j} + \frac{\partial h_i^{(3)}}{\partial y_j} \right) + K_{2ij}^{(1)} \left( \frac{\partial h_i^{(1)}}{\partial x_j} + \frac{\partial h_i^{(2)}}{\partial y_j} \right) + K_{2ij}^{(2)} I_{3j} \left] + \\
- \frac{\partial}{\partial x_i} \left[ K_{2ij}^{(0)} \left( \frac{\partial h_i^{(1)}}{\partial x_j} + \frac{\partial h_i^{(2)}}{\partial y_j} \right) + K_{2ij}^{(1)} \left( \frac{\partial h_i^{(0)}}{\partial x_j} + \frac{\partial h_i^{(1)}}{\partial y_j} \right) + K_{2ij}^{(1)} I_{3j} \right] = 0 \quad (3.97)
\]

The interface condition (3.76) at the order $\varepsilon^3$ gives on $\Gamma$:

\[
\left[ K_{1ij}^{(0)} \left( \frac{\partial h_i^{(2)}}{\partial x_j} + \frac{\partial h_i^{(3)}}{\partial y_j} \right) + K_{1ij}^{(1)} \left( \frac{\partial h_i^{(1)}}{\partial x_j} + \frac{\partial h_i^{(2)}}{\partial y_j} \right) + \right. \\
+ K_{1ij}^{(2)} \left( \frac{\partial h_i^{(0)}}{\partial x_j} + \frac{\partial h_i^{(1)}}{\partial y_j} \right) + K_{1ij}^{(2)} I_{3j} \left] N_i = \\
\left. \left[ K_{2ij}^{(0)} \left( \frac{\partial h_i^{(2)}}{\partial x_j} + \frac{\partial h_i^{(3)}}{\partial y_j} \right) + K_{2ij}^{(1)} \left( \frac{\partial h_i^{(1)}}{\partial x_j} + \frac{\partial h_i^{(2)}}{\partial y_j} \right) + K_{2ij}^{(2)} I_{3j} \right] N_i \quad (3.98)
\right]
\]

Now, let us integrate (3.96) over the sub-domain $\Omega_1$ and divide it by $|\Omega|$ and integrate (3.96) over the sub-domain $\Omega$ and divide it by $|\Omega|$. Then, add term by term the obtained equations. After the application of the divergence theorem, the condition (3.98) at the interface and the periodicity condition the following equation results:

\[
\left( \frac{1}{|\Omega_1|} \int_{\Omega_1} C_1^{(0)} d\Omega + \frac{1}{|\Omega_2|} \int_{\Omega_2} C_2^{(0)} d\Omega \right) \frac{\partial h^{(0)}}{\partial t^*} + \\
- \frac{1}{|\Omega|} \frac{\partial}{\partial x_i} \int_{\Omega_1} \left[ K_{1ij}^{(0)} \left( \frac{\partial h_i^{(1)}}{\partial x_j} + \frac{\partial h_i^{(2)}}{\partial y_j} \right) + \\
+ K_{1ij}^{(1)} \left( \frac{\partial h_i^{(0)}}{\partial x_j} + \frac{\partial h_i^{(1)}}{\partial y_j} \right) + K_{1ij}^{(2)} I_{3j} \right] d\Omega + \\
- \frac{1}{|\Omega|} \frac{\partial}{\partial x_i} \int_{\Omega_2} \left[ K_{2ij}^{(0)} \left( \frac{\partial h_i^{(1)}}{\partial x_j} + \frac{\partial h_i^{(2)}}{\partial y_j} \right) + K_{2ij}^{(1)} I_{3j} \right] d\Omega = 0 \quad (3.99)
\]
Using the relation (3.88) we can write (3.99) in a simplified form:

$$C_{\text{eff}} \frac{\partial h^{(0)}}{\partial t^*} - \frac{1}{|\Omega|} \frac{\partial}{\partial x_i} \int_{\Omega_i} \left[ K^{(0)}_{1ij} \left( \frac{\partial h^{(1)}}{\partial x_j} + \frac{\partial h^{(2)}}{\partial y_j} \right) \right] d\Omega + \frac{1}{|\Omega|} \frac{\partial}{\partial x_i} \int_{\Omega_2} \left[ K^{(0)}_{2ij} \left( \frac{\partial h^{(0)}}{\partial x_j} + \frac{\partial h^{(1)}}{\partial y_j} \right) + K^{(0)}_{2ij} I_3 \right] d\Omega = 0$$

(3.100)

where $C_{\text{eff}}$ is the effective water capacity, defined as:

$$C_{\text{eff}} = \frac{1}{|\Omega|} \int_{\Omega} C^{(0)}_1 d\Omega + \frac{1}{|\Omega|} \int_{\Omega_2} C^{(0)}_2 d\Omega = w_1 C^{(0)}_1 + w_2 C^{(0)}_2$$

(3.101)

Now, we will perform some transformations in order to put (3.100) in a form more suitable for practical application. Let us define the following fluxes:

$$q_{1i} = K^{(0)}_{1ij} \left( \frac{\partial h^{(1)}}{\partial x_j} + \frac{\partial h^{(2)}}{\partial y_j} \right)$$

(3.102)

$$q_{2i} = K^{(0)}_{2ij} \left( \frac{\partial h^{(0)}}{\partial x_j} + \frac{\partial h^{(1)}}{\partial y_j} \right) + K^{(0)}_{2ij} I_3$$

(3.103)

The second and third term in (3.100) contain volume integrals of these fluxes. The fluxes satisfy the following relations:

$$q_{1k} = \frac{\partial}{\partial y_k} (q_{1i} y_k)$$

(3.104)

$$q_{2k} = \frac{\partial}{\partial y_k} (q_{2i} y_k)$$

(3.105)

If the volume average of each flux is calculated and the divergence theorem is applied one obtains:

$$\frac{1}{|\Omega|} \int_{\Omega_1} q_{1k} d\Omega = -\frac{1}{|\Omega|} \int_{\Omega} \left[ K^{(0)}_{1ij} \left( \frac{\partial h^{(1)}}{\partial x_j} + \frac{\partial h^{(2)}}{\partial y_j} \right) \right] y_k N_i d\Gamma$$

(3.106)

$$\frac{1}{|\Omega|} \int_{\Omega_2} q_{2k} d\Omega = \frac{1}{|\Omega|} \int_{\Omega} \left[ K^{(0)}_{2ij} \left( \frac{\partial h^{(0)}}{\partial x_j} + \frac{\partial h^{(1)}}{\partial y_j} \right) + K^{(0)}_{2ij} I_3 \right] y_k N_i d\Gamma + \frac{1}{|\Omega|} \int_{\Lambda_k} \left[ K^{(0)}_{2ij} \left( \frac{\partial h^{(0)}}{\partial x_j} + \frac{\partial h^{(1)}}{\partial y_j} \right) + K^{(0)}_{2ij} I_3 \right] y_k N_i d\Lambda$$

(3.107)

where the unit normal vector $N$ is oriented outward to the sub-domain $\Omega_2$ and $\Lambda_k$ denotes the cross-section of $\Omega_2$ orthogonal to the $k$ direction. The flux continuity condition on $\Gamma$ at the order $\varepsilon^2$ has the form:

$$\left[ K^{(0)}_{1ij} \left( \frac{\partial h^{(1)}}{\partial x_j} + \frac{\partial h^{(2)}}{\partial y_j} \right) \right] N_i = \left[ K^{(0)}_{2ij} \left( \frac{\partial h^{(0)}}{\partial x_j} + \frac{\partial h^{(1)}}{\partial y_j} \right) + K^{(0)}_{2ij} I_3 \right] N_i$$

(3.108)
If the condition (3.108) is used, the sum of the averaged fluxes (3.106)–(3.107) can be written as a surface integral:

\[
\frac{1}{|\Omega|} \int_{\Omega_1} q_{1k} \, d\Omega + \frac{1}{|\Omega|} \int_{\Omega_2} q_{2k} \, d\Omega = \frac{1}{|\Omega|} \int_{\Lambda_k} \left[ K_{2ij}^{(0)} \left( \frac{\partial h^{(0)}}{\partial x_j} + \frac{\partial h_{2}^{(1)}}{\partial y_j} \right) + K_{2ij}^{(0)} I_{j\beta} \right] y_k N_i \, d\Lambda
\]

(3.109)

Finally, using equation (3.109) and the solution for \( h_2^{(1)} \) (3.90) the macroscopic equation is written as:

\[
C_{\text{eff}} \frac{\partial h^{(0)}}{\partial t} - \frac{\partial}{\partial x_i} \left[ K_{ij}^{\text{eff}} \frac{\partial}{\partial x_j} \left( h^{(0)} + x_3 \right) \right] = 0
\]

(3.110)

where the effective conductivity tensor \( K_{ij}^{\text{eff}} \) is defined as a surface integral:

\[
K_{ij}^{\text{eff}}(h^{(0)}) = \frac{1}{|\Lambda_i|} \int_{\Lambda_i} K_{2ik}(h^{(0)}) \left( I_{kj} - \frac{\partial \chi_j}{\partial y_k} \right) \, d\Lambda \quad i, j, k = 1, 2, 3
\]

(3.111)

The vector function \( \chi \) is the solution of the local boundary value problem (3.92)–(3.93). It can be demonstrated that \( K \) is symmetric and positively definite. If \( K_2 \) is isotropic and constant over the \( \Omega_2 \) sub-domain, (3.111) simplifies to:

\[
K_{ij}^{\text{eff}}(h^{(0)}) = \frac{K_2(h^{(0)})}{|\Lambda_i|} \int_{\Lambda_i} \left( I_{kj} - \frac{\partial \chi_j}{\partial y_k} \right) \, d\Lambda
\]

(3.112)

### 3.4.5 Discussion

The macroscopic model (3.110) is a single Richards-type equation, which includes capillary and gravity effects at the macroscopic scale. In this case local equilibrium conditions occur. The flow is controlled by the less conductive interconnected matrix \( \Omega_2 \). The effective conductivity is a function of the conductivity \( K_2 \) and the local geometry. It is independent of the inclusions conductivity \( K_1 \). The same results are obtained if the conductivity contrast is increased \( \frac{K_2}{K_1} < \varepsilon \). It has no influence on the form of macroscopic equation or the definition of the effective parameters.

The obtained model can be compared with the results presented by Panfilov et al. (1997) and Panfilov (2000). They studied two-phase flow in porous medium with highly permeable inclusions using asymptotic homogenization. It was shown, that local equilibrium exist, since the relaxation time for flow in inclusions is instantaneous, compared to flow in the less conductive matrix. The macroscopic absolute permeability and the relative phase permeabilities were shown to be independent of the permeability in inclusions. The parameters are calculated from the local boundary value problem analogous to (3.92)–(3.93). Thus, the results are similar to the model presented here.
Some other studies available in the literature (Levy, 1990; Moctezuma-Berthier et al., 2002; Moctezuma-Berthier A., 2004) refer to the fissured or vugular media and are based on different assumptions on the local scale physics (Stokes law in fissures/vugs). Nevertheless, they emphasize the influence of the connectivity of the highly permeable system on macroscopic properties of the medium. The same conclusion results from our analysis, since two very different models of flow were obtained, depending on the connectivity of the more conductive sub-domain.

3.5 Classification of the macroscopic models

In this section the results are compared with the model obtained by Lewandowska & Laurent (2001) using the same asymptotic homogenization technique. They assumed that the hydraulic conductivities and the capillary capacities are of the same order of magnitude in both sub-domains. The following macroscopic equation was obtained:

\[ C_{\text{eff}} \frac{\partial h(0)}{\partial t^*} - \frac{\partial}{\partial x_i} \left( K_{\text{eff}} \frac{\partial}{\partial x_j} (h(0) + x_3) \right) = 0 \]  

(3.113)

with the effective parameters \( C_{\text{eff}} \) and \( K_{\text{eff}} \) defined as:

\[ C_{\text{eff}}(h(0)) = w_1 C_1(0) + w_2 C_2(0) \]  

(3.114)

\[ K_{\text{eff}}^{ij}(h(0)) = \frac{1}{|\Omega|} \left( \int_{\Omega_1} K_1^{(0)}(I_{kj} + \frac{\partial \chi_I}{\partial y_k}) d\Omega_1 + \int_{\Omega_2} K_2^{(0)}(I_{kj} + \frac{\partial \chi_{II}}{\partial y_k}) d\Omega_2 \right) \]  

(3.115)

The vector function \( \chi \) is defined in both sub-domains. It is obtained from following local boundary value problem:

\[ \frac{\partial}{\partial y_i} \left[ K_1^{(0)} \left( I_{kj} + \frac{\partial \chi_I}{\partial y_k} \right) \right] = 0 \quad i, j, k = 1, 2, 3 \quad \text{in } \Omega_1 \]  

(3.116)

\[ \frac{\partial}{\partial y_i} \left[ K_2^{(0)} \left( I_{kj} + \frac{\partial \chi_{II}}{\partial y_k} \right) \right] = 0 \quad \text{in } \Omega_2 \]  

(3.117)

\[ \chi_I = \chi_{II} \quad \text{on } \Gamma \]  

(3.118)

\[ K_1^{(0)}(I_{kj} + \frac{\partial \chi_I}{\partial y_j}) N_i = K_{2kj}^{(0)} \left( I_{kj} + \frac{\partial \chi_{II}}{\partial y_j} \right) N_i \quad \text{on } \Gamma \]  

(3.119)

The superscripts \( I \) and \( II \) denote the function \( \chi \) in the \( \Omega_1 \) and \( \Omega_2 \) sub-domains, respectively. The function \( \chi \) satisfies has zero- valued average:

\[ \langle \chi \rangle = \frac{1}{|\Omega_1|} \int_{\Omega_1} \chi_I d\Omega + \frac{1}{|\Omega_2|} \int_{\Omega_2} \chi_{II} d\Omega = 0 \]  

(3.120)

and \( \chi \) is \( y \)-periodic. The effective conductivity depends on the local parameters \( K_1 \) and \( K_2 \).

In this case the connectivity of the more conductive sub-domain does not influence the form
of the model, since no large contrast of parameters exists. Similar results were obtained also
by other authors for one- and two-phase flow, using either asymptotic homogenization (Saez
et al., 1989; Amaziane et al., 1991) or the volume averaging method (Quintard & Whitaker,

3.5.1 Soil with weakly conductive inclusions

Comparing the macroscopic non-equilibrium model (3.63) to the equilibrium model (3.113)
one can note that there exists a continuous passage from (3.63) to (3.113).

First, we should note that the local problem defining effective conductivity (3.50)–(3.51)
in the non-equilibrium model can be considered as a limit case of the problem (3.116)–
(3.119). If the conductivity in inclusions \( K_2 \) tends to zero the inclusion becomes an inactive
obstacle for the flow and the condition (3.51) can be specified at the interface \( \Gamma \). Thus, one
obtains the problem (3.50)–(3.51).

Similarly we can examine the behavior of the nonlinear source term in equation (3.63).
The non-equilibrium model has been derived for the assumption that the characteristic time
of flow in inclusions at the local scale is of the same order as the time of flow in highly
conductive sub-domain at the macroscopic scale. If the conductivity ratio increases (from
\( \varepsilon^2 \) to 1), the time of flow in inclusions becomes shorter and shorter, compared to the time
of macroscopic phenomenon. Finally one can assume, that the pressure equilibration time
is comparable in the two sub-domains, which corresponds to the model (3.113)–(3.115).

Let us analyze the other possible situations, i.e. an intermediate case, when \( \frac{K_2}{K_1} = O(\varepsilon) \)
and the case of very high contrast \( \frac{K_2}{K_1} \leq O(\varepsilon^3) \). If the conductivity ratio is \( \frac{K_2}{K_1} = O(\varepsilon) \)
the solution of normalized equation leads to a model with local equilibrium (3.113), but
with macroscopic conductivity \( K_{eff} \) defined by the problem (3.50)–(3.51). It means that
the influence of \( K_2 \) becomes negligible, but the flow time in inclusions is much shorter than
in the macroscopic domain. For the observation time defined as the time of flow at the
macroscopic scale in more conductive sub-domain (3.27), local equilibrium exists.

Yet another situation arises when the conductivity ratio becomes much smaller than \( \varepsilon^2 \).
In such case the flow in inclusions is so slow, that we can consider them as impermeable.
The resulting equation is similar to (3.63), but the source term disappears. The medium
behaves as single-porosity system, with the effective parameters corresponding to the highly
conductive sub-domain.
Figure 3.2: Conditions at the interface $\Gamma$ in a double-porosity medium: (a) contrasting hydraulic conductivity, (b) and (c) contrasting capillary capacity.

3.5.2 Soils with highly conductive inclusions

Similarly to the previous case there exists a passage between the model (3.113) and the model for the soil with highly conductive inclusions (3.110). Let us assume that the conductivity in inclusions becomes much greater than in the matrix. In that case, the time required for equilibration of the pressure in inclusions will be very short compared to the equilibration time for matrix (at the local scale). Thus the local equilibrium in the less conductive matrix implies the equilibrium in inclusions.

The flow is determined entirely by the conductivity of the matrix and the local geometry. This analysis is valid for $\frac{K_2}{K_1} \leq O(\varepsilon)$. The local problem (3.92)–(3.93) obtained for such estimations represents a limit case of the problem (3.116)–(3.119) when $\frac{K_2}{K_1}$ in inclusions tends to infinity. As will be shown in Chapter 5, the values of $K_{eff}$ obtained from (3.92)–(3.93) are equal to those resulting from (3.116)–(3.119), when sufficiently small ratio $\frac{K_2}{K_1}$ is imposed. It confirms the consistency of the presented analysis.

3.5.3 Extension to the case of contrasting capillary capacity

In the preceding sections we have assumed that the capillary capacity of the two components is of the same order of magnitude ($\frac{C_1}{C_2} = O(1)$). Thus, the ratio of the capillary diffusivity was equal to the ratio of the hydraulic conductivity. In a more general case the capillary capacity may have different order in each sub-domain. Here we show, that the macroscopic models developed in this Chapter remains valid also in the case of contrasting capacities.

In order to illustrate this problem let us analyze conditions in the vicinity of the interface...
Γ between the sub-domains Ω₁ and Ω₂. First, let us assume that the capillary capacity is of the same order, while the hydraulic conductivity differs by ε² (Fig.3.2a), which is the case studied in Section 3.3 of this chapter. The pressure head is continuous at the interface. Due to the difference of the conductivity, the pressure gradient in Ω₂ is much larger than in Ω₁. In this way the fluxes are equal on both sides of the interface. Now, consider the situation when the two conductivities are similar, but the capacity ratio is \( \frac{C_1}{C_2} = \mathcal{O}(\varepsilon^2) \) (Fig.3.2b). It means that porous medium 1 has much more uniform pore-size distribution compared to medium 2. Note that the diffusivity ratio remains \( \frac{D_2}{D_1} = \mathcal{O}(\varepsilon^2) \). At a given time \( t \) we will have the same value of the water pressure head on both sides of the interface (due to the continuity condition) and two different values of water content, resulting from the retention curves for the two sub-domains. The pressure gradient is the same in both sub-domains, since \( K_1 = K_2 \). At the time \( t + \Delta t \) we will have the water pressure head \( h + \Delta h \), still the same on both sides. However, the increment of pressure head will cause very different increment of the water content in the two sub-domains. Since \( \frac{C_1}{C_2} = \mathcal{O}(\varepsilon^2) \) one obtains \( \Delta \theta_1 = C_1 \Delta h \ll \Delta \theta_2 = C_2 \Delta h \). This means that the mass balance at the interface is not satisfied — the volume of water which enters from one side is not equal to the volume leaving from the other side. Thus, the continuity of flux is not satisfied. If both continuity conditions have to be satisfied, one has to assume that in the sub-domain Ω₂ only a small boundary layer is influenced by the process (Fig.3.2b). The volume of this boundary layer should be chosen in such a manner, that the mass balance is satisfied. Locally, in the boundary layer the flux is the same as in the sub-domain Ω₁. However, if the pressure gradient is calculated with respect to the total considered volume of Ω₂ its value will be much smaller (Fig.3.2c). Thus, the scaling factor appear and the resulting normalized problem has the form equivalent to (3.32)–(3.35).

### 3.5.4 Catalogue of the macroscopic models

All the developed macroscopic models and their domain of validity are schematically presented in Fig. 3.3. Different models arise for the soils with highly conductive region connected and soils with highly conductive disconnected inclusions. The form of the model depends also on the ratio of the hydraulic parameters of the two sub-domains.

If the hydraulic parameters in the two sub-domains are of similar order of magnitude, one obtains the local-equilibrium model (). The effective parameters depends on the parameters of both components and on the local geometry. When the contrast of diffusivity increases, the form of the macroscopic model depends on the conductivity of the more conductive sub-domain.

If the conductivity of the interconnected sub-domain is increased with respect to the
Chapter 3. Development of the macroscopic models by homogenization

Figure 3.3: Macroscopic models of flow in heterogeneous soils and their domain of validity. Note that the effective capacities $C_{eff I}$ and $C_{eff II}$ and the effective conductivities $K_{eff I}$, $C_{eff III}$ and $K_{eff III}$ have different definitions.
inclusions we obtain first an intermediate model with local-equilibrium, then the local non-equilibrium model and finally an equilibrium simple porosity model, where the inclusions can be treated as impermeable. In all those models the effective conductivity depends only on the conductivity of the interconnected sub-domain and on the local geometry. In the first (intermediate) model the effective capacity depends on the capacities of the two sub-domains. In other models it depends on the capacity of the more conductive interconnected sub-domain. The influence of inclusions is either taken into account by the source term (non-equilibrium model) or it is neglected (simple porosity model).

For media with inclusions more conductive than the matrix the form of macroscopic model (local equilibrium) remains the same even for large contrast of diffusivity. However, when the local contrast of parameters increases, the definition of the effective conductivity tensor changes.

Finally, it should be stressed once again that the form of the macroscopic model is closely related to the choice of the observation time. Different models would be obtained if the definition of the characteristic time were changed.
Chapter 4

Numerical implementation of the macroscopic unsaturated flow models for double-porosity soils

4.1 Introduction

In the previous chapter the homogenization method was used to derive two distinct macroscopic models of the unsaturated flow in highly heterogeneous soils. A non-equilibrium model was obtained for the soils with the highly conductive sub-domain interconnected, when the ratio of the capillary diffusivity of the two components was of the order $O(\varepsilon^2)$. The macroscopic flow in soils with highly conductive disconnected inclusions is described by an equilibrium model. The practical application of each of the derived models involves two main stages:

1. Solution of the local boundary value problem (3.50)–(3.51) or (3.92)–(3.93) and calculation of the effective conductivity of the medium;

2. Solution of the macroscopic flow equation (3.63) or (3.110), which in case of the non-equilibrium flow is coupled with the solution of local flow in inclusions (3.55)–(3.56)

The solution process is generally outlined in Fig. 4.1. The required input information includes the local geometry of the period and the hydraulic characteristics of the two sub-domains. The data allow to calculate the effective parameters of the double-porosity medium. The macroscopic equation is then solved for the specified initial and boundary conditions. Both stages require the use of numerical methods, since analytic solutions of the concerned equations are not available (except for some particular cases). For the purposes of this study a numerical code DPOR-1D has been developed (see also Lewandowska et al. (2004b)). It
Chapter 4. Numerical implementation of the macroscopic flow models

Figure 4.1: General strategy of the application of the macroscopic flow model obtained by homogenization.

The macroscopic flow is assumed to be one-dimensional. The one-dimensional form of the flow equation is commonly used in the unsaturated zone modeling and may be applied to simulate field-scale problems as well as the flow in laboratory columns.

In contrast, the local geometry is three-dimensional, which allows to account for various types of soil structure (Fig. 4.2). The geometries implemented in the DPOR-1D code include:

1. Vertical slabs of more conductive and less conductive medium parallel to the direction
Chapter 4. Numerical implementation of the macroscopic flow models

Figure 4.2: Period geometries implemented in DPOR.1D: (I) vertical slabs, (II) vertical columns, (III) cylinders, (IV) horizontal columns, (V) spheres (simple arrangement), (VI) parallelepipeds (simple arrangement), (VII) spheres (centered arrangement), (VIII) parallelepipeds (centered arrangement).

1. One-dimensional inclusions of macroscopic flow, Fig. 4.2-I;

2. Vertical columns of more conductive medium in less conductive matrix, Fig. 4.2-II;

3. Two-dimensional inclusions in form of circle, representing infinite horizontal cylinders, Fig. 4.2-III;

4. Two-dimensional inclusions in form of rectangle, representing infinite horizontal columns, Fig. 4.2-IV;

5. Three-dimensional inclusions in form of sphere in simple or centered arrangement, Fig. 4.2-V,VII;

6. Three-dimensional inclusions in form of parallelepiped in simple or centered arrangement, Fig. 4.2-VI,VIII.

Note that for the geometry I, III V and VII the local flow in inclusions can be described by one-dimensional equation in orthogonal or radial coordinates. For the geometry II or III the local flow is two-dimensional, while for geometry VI and VIII — three-dimensional. For
the medium with highly conductive inclusions only geometries are possible with the more conductive sub-domain $\Omega_1$ disconnected are possible (III to VI).

We assumed that both sub-domains are locally homogeneous and isotropic. Thus, the hydraulic conductivities of the highly conductive and the weakly conductive component of the medium are scalar values, which will be denoted by $K_1$ and $K_2$, respectively.

Each of the two sub-domains is characterized by the constitutive relations $\theta(h)$ and $K(h)$. Four models of the hydraulic functions are implemented in DPOR-1D:

- van Genuchten – Mualem functions (2.17) and (2.22)
- Brooks – Corey functions (2.16) and (2.20)
- van Genuchten retention function (with Burdine condition) (2.17) and Brooks – Corey conductivity function (2.20)
- user defined functions in tabularized form, the values between points are calculated by linear interpolation.

## 4.3 Calculation of the effective parameters

According to the results of homogenization, the effective water capacity is defined as a linear function of the capacities of the two regions $C_1$ and $C_2$:

\[
C_{\text{eff}} (h) = w_1 C_1 (h)
\]

for the non-equilibrium flow or:

\[
C_{\text{eff}} (h) = w_1 C_1 (h) + w_2 C_2 (h)
\]

for the equilibrium flow, where $w_1$ and $w_2$ are the volume fractions of two sub-domains. Note that the variables in (4.1) and (4.2) are dimensional. The calculation of the average water content and the effective water capacity is straightforward and requires only the information on $w_1$ and $w_2$.

All considered soil structures are symmetric with respect to the axes $y_1$, $y_2$ and $y_3$, thus the components outside the main diagonal are equal to zero. The effective conductivity coefficient is a symmetrical second rank tensor:

\[
K_{\text{eff}} = \begin{bmatrix}
K_{11} & 0 & 0 \\
0 & K_{22} & 0 \\
0 & 0 & K_{33}
\end{bmatrix}
\]
Since we assume that the macroscopic flow is one-dimensional and occurs in $y_3$ direction, the only required component of the effective tensor is $K_{33}^{eff}$, which from now on will be denoted by $K^{eff}$.

The numerical approach to the solution of the local boundary value problem has been partially inspired by MONO3D code of Quintard (1997).

### 4.3.1 Soil with weakly conductive inclusions

The effective conductivity of the double-porosity medium is defined as:

\[
K^{eff}(h) = K_1(h) \left| \Omega_1 \right| \int_{\Omega_1} \left( 1 + \frac{\partial \chi_3}{\partial y_3} \right) d\Omega \tag{4.3}
\]

which can be rewritten in a shortened form as:

\[
K^{eff}(h) = K_E K_1(h) \tag{4.4}
\]

Note that $K^{eff}$ and $K_1$ are now dimensional variables. The dimensionless constant coefficient $K_E$ represents the influence of the geometry of the medium. The $\chi_3$ component of the vector function $\chi$, required for the calculation of $K_E$, is obtained from the following dimensionless local boundary problem (resulting from (3.50)–(3.51)):

\[
\frac{\partial}{\partial y_1} \left[ K_1^{(0)} \left( \frac{\partial \chi_3}{\partial y_1} \right) \right] + \frac{\partial}{\partial y_2} \left[ K_1^{(0)} \left( \frac{\partial \chi_3}{\partial y_2} \right) \right] + \frac{\partial}{\partial y_3} \left[ K_1^{(0)} \left( 1 + \frac{\partial \chi_3}{\partial y_3} \right) \right] = 0 \text{ in } \Omega_1 \tag{4.5}
\]

with the condition:

\[
\left[ K_1^{(0)} \left( \frac{\partial \chi_3}{\partial y_1} \right) \right] N_1 + \left[ K_1^{(0)} \left( \frac{\partial \chi_3}{\partial y_2} \right) \right] N_2 + \left[ K_1^{(0)} \left( 1 + \frac{\partial \chi_3}{\partial y_3} \right) \right] N_3 = 0 \text{ on } \Gamma \tag{4.6}
\]

Moreover the function $\chi_3$ should satisfy the periodicity conditions and its volume average over $\Omega$ should be equal to zero.

The interface $\Gamma$ represents the boundary surface between the two sub-domains, which in general has an irregular shape. In order to simplify the numerical implementation we decided to solve an equivalent problem defined over the whole period. As it is shown in the previous chapter, the problem (4.3)–(4.5) can be replaced by an equivalent problem defined
Figure 4.3: Spatial discretization of the three-dimensional domain for the solution of the local boundary value problem.

over both sub-domains (3.116)–(3.119):

\[
\frac{\partial}{\partial y_i} \left[ K^{(0)}_{1ij} \left( I_{jk} + \frac{\partial \chi^I_k}{\partial y_j} \right) \right] = 0 \quad i, j, k = 1, 2, 3 \quad \text{in } \Omega_1 \quad (4.7)
\]

\[
\frac{\partial}{\partial y_i} \left[ K^{(0)}_{1ij} \left( I_{jk} + \frac{\partial \chi^{II}_k}{\partial y_j} \right) \right] = 0 \quad \text{in } \Omega_2 \quad (4.8)
\]

\[\chi^I_i = \chi^{II}_i \quad \text{on } \Gamma \quad (4.9)\]

\[
K^{(0)}_{1ij} \left( I_{jk} + \frac{\partial \chi^I_k}{\partial y_j} \right) N_i = K^{(0)}_{2ij} \left( I_{jk} + \frac{\partial \chi^{II}_k}{\partial y_j} \right) N_i \quad \text{on } \Gamma \quad (4.10)
\]

where \(K^{(0)}_{2}\) denote the conductivity of the weakly conductive inclusions. The two problems are equivalent when the conductivity contrast is large. In our calculations we assumed that \(K^{(0)}_{1} = 1\) and \(K^{(0)}_{2} = 10^{-15}\). Note that the solution of (4.5)–(4.6) is independent of the dimensionless conductivity \(K^{(0)}_{1}\).

Equation (4.5) with the condition (4.6) represents a Poisson type elliptic problem. Numerical solution of such problems has been widely studied in literature e.g. (Björck & Dahlquist, 1974; Press et al., 1996). In DPOR-1D the finite difference method was used to solve the equation (4.5). We are aware of some shortcomings of this method, concerning the discretization of non-rectangular geometries and the approximation of fluxes. However, numerical tests showed that it performs well for simple geometries considered in this study (see Chapter 5).

We assume that the period has the form of a rectangular parallelepiped of the dimensions
$l_1 \times l_2 \times l_3$ in $y_1$, $y_2$ and $y_3$ directions respectively, see Fig. 4.3. The $(0,0,0)$ point corresponds to the center of the parallelepiped. The solution domain is discretized with a regular grid of $N = N_1 \times N_2 \times N_3$ nodes. Numerical approximation of (4.5) with finite differences yields:

$$\frac{q_{i+1/2,\kappa,\lambda} - q_{i-1/2,\kappa,\lambda}}{\Delta y_1} + \frac{q_{i,\kappa+1/2,\lambda} - q_{i,\kappa-1/2,\lambda}}{\Delta y_2} + \frac{q_{i,\kappa,\lambda+1/2} - q_{i,\kappa,\lambda-1/2}}{\Delta y_3} = 0$$  \hspace{1cm} (4.11)

where $i, \kappa, \lambda$ are node indices related to the $y_1$, $y_2$ and $y_3$ directions respectively and $\Delta y_1$, $\Delta y_2$ and $\Delta y_3$ denote distance between nodes in the respective directions. The fluxes $q$ are approximated by the following differential formulas:

$$q_{i+1/2,\kappa,\lambda} = K_{i+1/2,\kappa,\lambda} \frac{\chi_{i+1,\kappa,\lambda} - \chi_{i,\kappa,\lambda}}{\Delta y_1}$$  \hspace{1cm} (4.12)

$$q_{i-1/2,\kappa,\lambda} = K_{i-1/2,\kappa,\lambda} \frac{\chi_{i-1,\kappa,\lambda} - \chi_{i,\kappa,\lambda}}{\Delta y_1}$$  \hspace{1cm} (4.13)

$$q_{i,\kappa+1/2,\lambda} = K_{i,\kappa+1/2,\lambda} \frac{\chi_{i,\kappa+1,\lambda} - \chi_{i,\kappa,\lambda}}{\Delta y_2}$$  \hspace{1cm} (4.14)

$$q_{i,\kappa-1/2,\lambda} = K_{i,\kappa-1/2,\lambda} \frac{\chi_{i,\kappa-1,\lambda} - \chi_{i,\kappa,\lambda}}{\Delta y_2}$$  \hspace{1cm} (4.15)

$$q_{i,\kappa,\lambda+1/2} = K_{i,\kappa,\lambda+1/2} + K_{i,\kappa,\lambda+1/2} \frac{\chi_{i,\kappa,\lambda+1} - \chi_{i,\kappa,\lambda}}{\Delta y_3}$$  \hspace{1cm} (4.16)

$$q_{i,\kappa,\lambda-1/2} = K_{i,\kappa,\lambda-1/2} + K_{i,\kappa,\lambda-1/2} \frac{\chi_{i,\kappa,\lambda-1} - \chi_{i,\kappa,\lambda}}{\Delta y_3}$$  \hspace{1cm} (4.17)

where $K_{i,\pm1/2}$ is the mean conductivity in the considered grid block calculated as an arithmetic average. The subscript 3 at $\chi$ is omitted for simplicity.

For the symmetric geometries considered here the periodic boundary conditions can be imposed in the following straightforward manner (Auriault & Lewandowska, 2001):

- for the boundaries normal to the flow direction, the Dirichlet condition is imposed:

$$\chi_3 = 0 \hspace{0.5cm} \text{for} \hspace{0.5cm} y_3 = -l_3/2 \hspace{0.5cm} \text{and} \hspace{0.5cm} y_3 = l_3/2$$  \hspace{1cm} (4.18)

- for the boundaries parallel to the flow direction, the zero-flux condition is imposed:

$$\frac{\partial \chi_3}{\partial y_1} = 0 \hspace{0.5cm} \text{for} \hspace{0.5cm} y_1 = -l_1/2 \hspace{0.5cm} \text{and} \hspace{0.5cm} y_1 = l_1/2$$  \hspace{1cm} (4.19)

$$\frac{\partial \chi_3}{\partial y_2} = 0 \hspace{0.5cm} \text{for} \hspace{0.5cm} y_2 = -l_2/2 \hspace{0.5cm} \text{and} \hspace{0.5cm} y_2 = l_2/2$$  \hspace{1cm} (4.20)

Finally, a system of $N$ linear algebraic equations is obtained, which can be written in a matrix form as:

$$A \chi = b$$  \hspace{1cm} (4.21)

where $A$ is the coefficient matrix, $\chi$ is the unknown vector of values of $\chi_3$ in nodes and $b$ is the right hand side vector. The system is solved by successive over-relaxation (SOR) method.
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(see section 4.3.3). The solution yields the values of unknown function \( \chi_3 \) at all nodes. The \( K_E \) coefficient is then calculated as the integral from (4.3). For the purpose of numerical integration the function \( \chi \) between nodes is approximated by linear interpolation.

One should note that for the particular local geometries, where region \( \Omega_1 \) has form of layers or columns parallel to the flow direction (geometry I or II, Fig.4.2) the solution of (4.5)–(4.6) can be done analytically and yields:

\[
\chi_3 = 0 \quad \text{and} \quad \frac{\partial \chi_3}{\partial y_3} = 0 \quad (4.22)
\]

and consequently:

\[
K_E = w_1 \quad (4.23)
\]

In other cases the effective coefficient \( K_E \) is smaller than the volume fraction \( w_1 \). Examples of calculation of the effective conductivity are presented in Chapter 5.

4.3.2 Soil with highly conductive inclusions

In the medium with highly conductive inclusions the \( K^{eff}_{33} \) component of the effective conductivity tensor is defined as:

\[
K^{eff}_{33}(h) = \frac{K_2^{(0)}(h)}{2} \int_{\Lambda_3} \left( 1 - \frac{\partial \chi_3}{\partial y_3} \right) d\Lambda \quad (4.24)
\]

where \( \Lambda_3 \) is the cross-section surface of the period perpendicular to the \( y_3 \) direction. Similarly to the previous case (4.24) can be represented in a shortened form:

\[
K^{eff}(h) = K_E K_2(h) \quad (4.25)
\]

The function \( \chi_3 \) is the solution of the following local boundary value problem (resulting from (3.92)–(3.93)):

\[
\frac{\partial}{\partial y_1} \left[ K_2^{(0)} \left( - \frac{\partial \chi_3}{\partial y_1} \right) \right] + \frac{\partial}{\partial y_2} \left[ K_2^{(0)} \left( - \frac{\partial \chi_3}{\partial y_2} \right) \right] + \frac{\partial}{\partial y_3} \left[ K_2^{(0)} \left( 1 - \frac{\partial \chi_3}{\partial y_3} \right) \right] = 0 \quad \text{in} \ \Omega_2
\]

with the boundary condition:

\[
\chi_3 = y_3 \quad \text{on} \ \Gamma \quad (4.27)
\]

Similarly to the previous case the function \( \chi_3 \) is \( y \)-periodic. Since the solution is independent of \( K_2^{(0)} \) it is assumed \( K_2^{(0)} = 1 \). The discretization is performed in the same way as described
in previous section. For each node in the region \( \Omega_2 \) the discrete analog of (4.26) similar to (4.11) is written:

\[
-\frac{q_{i+1/2,\kappa,\lambda} - q_{i-1/2,\kappa,\lambda}}{\Delta y_1} - \frac{q_{i,\kappa+1/2,\lambda} - q_{i,\kappa-1/2,\lambda}}{\Delta y_2} + \frac{q_{i,\kappa,\lambda+1/2} - q_{i,\kappa,\lambda-1/2}}{\Delta y_3} = 0 \tag{4.28}
\]

where:

\[
q_{i,\kappa,\lambda+1/2} = K_{i,\kappa,\lambda+1/2} - K_{i,\kappa,\lambda+1/2} \frac{\chi_{i,\kappa,\lambda+1} - \chi_{i,\kappa,\lambda}}{\Delta y_3} \tag{4.29}
\]

\[
q_{i,\kappa,\lambda-1/2} = K_{i,\kappa,\lambda-1/2} - K_{i,\kappa,\lambda-1/2} \frac{\chi_{i,\kappa,\lambda} - \chi_{i,\kappa,\lambda-1}}{\Delta y_3} \tag{4.30}
\]

The fluxes in other directions are defined according to (4.12)–(4.15). At the nodes corresponding to the \( \Omega_1 \) part of the period a Dirichlet condition is imposed:

\[
\chi_{i,\kappa,\lambda} = y_3
\]

In this way the condition at the interface \( \Gamma \) (4.27) is satisfied. Periodic boundary conditions are applied at the outer boundaries of the period, as described above ((4.18)–(4.20)). After the solution of the global system of equations the integral in (4.24) is calculated numerically, the function \( \chi_3 \) between nodes being interpolated linearly.

The effective coefficient \( K_E \) is greater than 1. Its value tends to infinity as \( w_2 \) tends to 0. Examples of the calculations can be found in Chapter 5.

4.3.3 Solution of sparse linear systems

The discretization of problem (4.5)–(4.6) or (4.26)–(4.27) leads to a large system of \( N = N_1 \times N_2 \times N_3 \) linear equations. The coefficient matrix \( A \) is banded and very sparse. In each row maximum 7 non-zero elements may appear. Such problems are most effectively solved with an iterative method. In our case the successive over-relaxation method (SOR) was applied (Fletcher, 1991; Björck & Dahlquist, 1974). The scheme of the method is following:

\[
\chi_i^{(k+1)} = \chi_i^{(k+1)} + \omega r_i^{(k)} \tag{4.31}
\]

where: \( k \) denotes the iteration index, \( \omega \) is the relaxation coefficient \( \chi_i \) is the \( i \)-th component of unknown vector and \( r_i \) is \( i \)-th component of residual vector. The elements of the vector \( r \) are calculated from the formula:

\[
r_i^{(k)} = \frac{1}{a_{ii}} \left( b_i - \sum_{j=1}^{i-1} a_{ij} \chi_j^{(k+1)} - \sum_{j=i}^{N} a_{ij} \chi_j^{(k)} \right) \tag{4.32}
\]

where \( a_{ij} \) and \( b_i \) denote the elements of the coefficient matrix and the right-hand side vector respectively. In our case the first approximation of the solution is \( \chi^{(0)} = 0 \). The iterative
process is continued until the specified accuracy of the solution is reached:

$$\| r \| \leq N \tau_{SOR}$$  \hspace{1cm} (4.33)

where $\tau_{SOR}$ is the required accuracy of the solution.

The norm $\| r \|$ is defined as:

$$\| r \| = \left( \sum_{i=1}^{N} r_i^2 \right)^{1/2}$$  \hspace{1cm} (4.34)

Numerical experiments showed that good results are obtained with the accuracy $\tau_{SOR} = 10^{-12}$ and the relaxation coefficient $\omega = 1.9$, which were used in the examples presented in next chapter.

### 4.4 Solution of the macroscopic equation

The two macroscopic equations derived by the method of homogenization (3.63) and (3.110) can be rewritten in the following one-dimensional form:

$$\frac{\partial \theta}{\partial t} - \frac{\partial}{\partial X} \left( K \frac{\partial h}{\partial X} - \nu K \right) + Q = 0$$  \hspace{1cm} (4.35)

In equation (4.35) we have replaced the dimensionless variables by the dimensional variables. Since the flow is one-dimensional, the space variable is a scalar denoted by $X$. The direction of the flow can be vertical, horizontal or inclined, which is taken into account by the coefficient $\nu$ ($\nu = 0$ for horizontal flow, $\nu = 1$ for vertical flow). Note that for vertical flow the spatial variable $X$ is oriented positively downward. $K$ is the effective conductivity (for the simplicity of notation we omit the superscript). Note that the retention term is now expressed in terms of the volumetric water content rather than the water pressure head. It has been shown (Celia et al., 1990) that such formulation has better numerical properties (mass conservation). In equation (4.35) $\theta$ has different meaning depending on the considered macroscopic model. In the case of the non-equilibrium flow it is defined as:

$$\theta = w_1 \theta_1$$  \hspace{1cm} (4.36)

and for the equilibrium flow as:

$$\theta = w_1 \theta_1 + w_2 \theta_2$$  \hspace{1cm} (4.37)

The source term $Q = Q(h)$ appears only in the non-equilibrium model and is defined as:

$$Q = \frac{1}{|\Omega|} \int_{\Omega_2} C_2 \frac{\partial h_2}{\partial t} d\Omega = \frac{1}{|\Omega_2|} \int_{\Omega_2} \frac{\partial \theta_2}{\partial t} d\Omega$$  \hspace{1cm} (4.38)
where $\theta_2$, $C_2$ and $h_2$ denote respectively the local volumetric water content, the capillary capacity and the water pressure head in the weakly conductive inclusions $\Omega_2$.

The equation (4.35) is a partial differential equation of parabolic type. It is highly nonlinear due to the dependency of $\theta$, $K$ and $Q$ on the macroscopic water pressure head $h$. Moreover, the solution of local and global flow problems is coupled. The numerical solution of such problem requires a special approach. Each node of the macroscopic grid is associated with a representative period (Fig. 4.4). The flow in weakly conductive inclusion is described by a local-scale equation (with respect to the spatial variable $Y$). The macroscopic and local equations are coupled by the condition of the pressure continuity at the interface $\Gamma$. Thus the solution domain consists of a one-dimensional macroscopic domain and a series of three-dimensional domains representing the inclusions. The number of inclusions corresponds to the number of macroscopic nodes and in general it is different from the real number of inclusions in the considered soil profile.

The solution of the macroscopic equation can be split into several steps. First, the spatial discretization of (4.35) is made. Consequently, the partial differential equation is transformed into a system of ordinary differential equations with respect to time (each equation corresponds to a single node of the numerical grid). Then, the discretization in time is performed. At each time level one obtains a system of highly nonlinear algebraic equations with respect to pressure head $h$. The nonlinear system is solved by an iterative method. This stage involves the solution of the local-scale flow in inclusions, in order to update the source term $Q$. Finally, in each iteration a linear algebraic system arises. The solution of this system gives the sought values of water pressure head. In the following paragraphs we present the successive stages of the solution.

### 4.4.1 Initial and boundary conditions

The equation (4.35) is solved in the domain $0 \leq X \leq L$ for specified initial and boundary conditions. The initial condition defines the distribution of pressure head (or water content) in the profile at the starting time. Since there are two pressure fields — macroscopic $h(X,t)$ and local $h_2(X,Y,t)$, the initial condition should be specified for each of them:

$$h(X,t = 0) = h_{\text{init}}(X)$$

$$h_2(X,Y,t = 0) = h_{\text{init}}(X)$$

Three types of boundary conditions were used in the numerical calculations with DPOR-1D code presented in this study:
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solution domain of the macroscopic equation (1D)

\[
\frac{\partial \theta}{\partial t} - \frac{\partial}{\partial X} \left( K \frac{\partial h}{\partial X} - K \right) + \int_{\Omega} \frac{\partial \theta}{\partial t} \, d\Omega = 0
\]

solution domains of the local equations (3D)

\[
\frac{\partial \theta}{\partial t} - \frac{\partial}{\partial Y} \left( K \frac{\partial h}{\partial Y} \right) = 0
\]

1. Dirichlet type condition — a specified value of pressure head was imposed at the top or bottom of the profile:

\[
h(X = 0, t) = h_{\text{surf}}(t) \quad \text{or} \quad h(X = L, t) = h_{\text{bot}}(t)
\]

2. Neuman type condition — a specified value of flux is imposed at the top or bottom of the profile:

\[
\left[ -K \frac{\partial h}{\partial X} + K \right]_{X=0} = q_{\text{surf}}(t) \quad \text{or} \quad \left[ -K \frac{\partial h}{\partial X} + K \right]_{X=L} = q_{\text{bot}}(t)
\]

3. Gradient type condition — this condition appears when free drainage is assumed at the bottom of the soil profile:

\[
\left. \frac{\partial h}{\partial t} \right|_{X=L} = 0 \quad \text{and consequently} \quad q_{\text{bot}} = K
\]

Figure 4.4: Coupled solution of macroscopic and local equations in the non-equilibrium flow model.


4.4.2 Discretization in space

Spatial discretization of (4.35) is performed with finite difference method (FDM) on a uniform grid of \( N \) nodes. It leads to the following semi-discrete form of equation:

\[
\frac{d\theta}{dt}\bigg|_{i} + \frac{q_{i+1/2} - q_{i-1/2}}{\Delta X} + Q_i = 0 \tag{4.39}
\]

where \( i \) is the node index \((i = 1 \ldots N)\), \( \Delta X \) is the spatial interval and \( q_{i+1/2} \) and \( q_{i-1/2} \) are the fluxes between nodes. The fluxes are approximated as:

\[
q_{i-1/2} = -K_{i-1/2} \frac{h_i - h_{i-1}}{\Delta X} + K_{i-1/2} \tag{4.40}
\]

\[
q_{i+1/2} = -K_{i+1/2} \frac{h_{i+1} - h_i}{\Delta X} + K_{i+1/2} \tag{4.41}
\]

The conductivities between nodes are approximated as arithmetic means:

\[
K_{i\pm 1/2} = \frac{1}{2} (K_{i+1} + K_i) \tag{4.42}
\]

Note that the same result can be obtained when applying finite element (FEM) discretization with linear shape functions and lumping of the mass coefficient matrix (Celia et al., 1990). Several other propositions for estimating the average conductivities can be found in (Haverkamp et al., 1977; Miller et al., 1998). The geometric mean was found to be more accurate than the arithmetic mean (Haverkamp & Vauclin, 1979), while the best results are obtained by integration of \( K(h) \) function in the interval \((h_i, h_{i\pm 1})\) (Miller et al., 1998). On the other hand the influence of the method of approximation becomes insignificant for small values of \( \Delta X \) (van Dam & Feddes, 2000).

4.4.3 Discretization in time

Discretization in time is performed with a differential scheme of the following form:

\[
\frac{\theta_i^{j+1} - \theta_i^j}{\Delta t^j} = \xi \frac{d\theta}{dt}\bigg|_{i}^{j+1} + (1 - \xi) \frac{d\theta}{dt}\bigg|_{i}^{j} \tag{4.43}
\]

where \( j \) is the time level index, \( \Delta t^j \) is the time step size (variable during the solution) and \( \xi \) is the weighting parameter which may assume values from 0 to 1. Note that \( \xi = 0 \) corresponds to the explicit Euler scheme, \( \xi = 0.5 \) to the Crank-Nicholson scheme and \( \xi = 1 \) to the fully implicit scheme. To ensure the stability of the solution \( \xi \) should not be less than 0.5 (Quarteroni & Valli, 1997; Fletcher, 1991). Application of the scheme (4.43) to the equation (4.35) for an internal node \( i \) leads to the following discretized equation:

\[
\frac{\theta_i^{j+1} - \theta_i^j}{\Delta t^j} + \xi \left[ \frac{q_{i+1/2}^{j+1} - q_{i-1/2}^{j+1}}{\Delta X} + Q_{i+1}^{j+1} \right] + (1 - \xi) \left[ \frac{q_{i+1/2}^j - q_{i-1/2}^j}{\Delta X} + Q_i^j \right] = 0 \tag{4.44}
\]
Note that the exchange term $Q$ is treated implicitly. In the preliminary tests we examined the explicit treatment of $Q$, i.e. the values of the exchange term in the macroscopic equation were taken from the previous time level. Such approach reduced the computational effort, however it led to unstable solution. Thus, we decided to treat $Q$ in an implicit manner, which is much more efficient.

At the boundary nodes appropriate conditions should be implemented:

- for Dirichlet condition (specified pressure head) the equations are simply:

$$h_j^{i+1} = h_{b0}^j$$ (4.45)

for the first (top) node and:

$$h_N^{i+1} = h_{bL}^j$$ (4.46)

- the implementation of prescribed flux yields:

$$\frac{\theta_i^{j+1} - \theta_i^j}{\Delta t} + \xi \left[ \frac{q_i^{j+1} - q_i^j}{\Delta x} + Q_i^{j+1} \right] + (1 - \xi) \left[ \frac{q_{i+1/2}^j - q_i^j}{\Delta x} + Q_i^j \right] = 0$$ (4.47)

for the first node and:

$$\frac{\theta_i^{j+1} - \theta_i^j}{\Delta t} + \xi \left[ \frac{q_{bL}^j - q_{N-1/2}^j}{\Delta x} + Q_N^{j+1} \right] + (1 - \xi) \left[ \frac{q_{bL}^j - q_{N-1}^j}{\Delta x} + Q_N^j \right] = 0$$ (4.48)

for the last node, where $q_{b1}$ and $q_{bN}$ are prescribed flux values;

- for free drainage condition at the bottom node we have:

$$\frac{\theta_i^{j+1} - \theta_i^j}{\Delta t} + \xi \left[ \frac{K_N^{j+1} - q_{i-1/2}^j}{\Delta x} + Q_i^{j+1} \right] + (1 - \xi) \left[ \frac{K_N^{j} - q_{i-1/2}^j}{\Delta x} + Q_i^j \right] = 0$$ (4.49)

The equation (4.44) is written for all internal nodes, $i = 2, \ldots, N - 1$. Including the appropriate equations for boundary nodes one obtains a system of N algebraic equations. The system is highly nonlinear. The water content $\theta^{j+1}$, effective conductivity $K^{j+1}$, water fluxes and source term $Q^{j+1}$ appearing in (4.44)–(4.49) are nonlinear functions of the macroscopic pressure head at the new time level $h^{j+1}$. Thus, the system can be written in the following abbreviated form:

$$f_i(h^{j+1}) = 0$$ (4.50)

where $f_i$ represents the equation (4.44) for $i = 2, \ldots, N - 1$, or one of the equations (4.45)–(4.49) for $i = 1$ and $i = N$. The unknown vector $h^{j+1}$ represents the nodal values of pressure head at the new time level.
4.4.4 Solution of the nonlinear systems

The system of nonlinear equations (4.50) should be solved by an iterative method. Both Picard and Newton schemes are used in the unsaturated flow modeling. The Picard method seems to be more widespread, since it requires less computational effort. Our preliminary tests showed that the Picard method performs well when \( Q = 0 \) in the macroscopic equation (4.35), but it is unstable when the non-equilibrium term \( Q \) is present. Thus, we have chosen the Newton method. Its scheme is following:

\[
J^{(k)} \Delta h^{(k+1)} = -f^{(k)}
\]

\[
h^{(k+1)} = h^{(k)} + \Delta h^{(k+1)}
\]

where: \((k)\) denotes iteration index, \( k = 0, \ldots, m \), \( J \) is the jacobian matrix and \( \Delta h \) is the increment of the unknown vector. The partial derivatives in jacobian matrix are approximated numerically with the following formula:

\[
J_{ij} = \frac{\partial f_i}{\partial h_j} = \frac{f_i(h_j + \sigma) - f_i(h_j)}{\sigma}
\]

where \( \sigma \) is a small parameter. The value of \( \sigma \) should be chosen according to the numerical conditions and the machine precision. In our calculations good results were obtained with \( \sigma = 10^{-4} \). Similarly to the coefficient matrix, the jacobian matrix is tridiagonal. Each internal row contains three non-zero elements: \( J_{i,i-1} \), \( J_{i,i} \) and \( J_{i,i+1} \). The elements in the first and last row depend on the form of the imposed boundary conditions.

It should be noted that the derivative of the source term \( \frac{\partial Q}{\partial h} \) is especially tedious to compute, as it requires that local flow equation is solved twice for each node. In order to decrease the computational effort a simplified approach can be used, where the derivative is computed in the first iteration only and used successively in subsequent iterations. The values of the source term are updated according to the following formula:

\[
Q_i^{j+1,(k)} = Q_i^{j+1,(0)} + \frac{\partial Q}{\partial h}\bigg|_{i_j} \left( h_i^{j+1,(k)} - h_i^{j+1,(0)} \right)
\]

Similar algorithm was presented by Arbogast (1997) for single-phase and two-phase flow in fractured media. In the program DPOR-1D the source term can be either evaluated using the simplified approach (4.54) or it can be calculated in each iteration from the solution of the local flow equations in inclusions.

In order to obtain the values of \( \Delta h \) in each iteration the system of linear equations (4.51) should be solved. The iterative process is terminated when the changes in the solution between two subsequent iterations become sufficiently small. The termination criterion is defined as:

\[
\Delta h_i^k \leq \tau_{IT}^{ABS} + \tau_{IT}^{REL} |h_i^k|
\]
where $\tau^{ABS}_{IT}$ and $\tau^{REL}_{IT}$ — absolute and relative tolerance for iterative solution. Note that they should be smaller than the tolerances imposed on the temporal truncation error (see section 4.4.5). For our calculation $\tau^{ABS}_{IT} = 0.5 \tau^{ABS}$ and $\tau^{REL}_{IT} = 0.5 \tau^{REL}$ was set. To ensure the convergence of the iterative process, the first approximation of the solution should be close enough to the exact solution. The following formula was used to calculate the first approximation at the new time level $j + 1$ (Kavetski et al., 2001):

$$ h^{j+1,0} = h^j + \frac{\partial h}{\partial t} |^j \Delta t^j + \frac{\partial^2 h}{\partial t^2} |^j (\Delta t^j)^2 $$  \hspace{1cm} (4.56)

The derivatives of $h$ with respect to time appearing in (4.56) are approximated with the backward finite differences:

$$ \frac{\partial h}{\partial t} |^j = \frac{h^j - h^{j-1}}{\Delta t^{j-1}} $$  \hspace{1cm} (4.57)

$$ \frac{\partial^2 h}{\partial t^2} = \frac{1}{\Delta t^{j-1}} \left( \frac{\partial h}{\partial t} |^j - \frac{\partial h}{\partial t} |^j^{j-1} \right) $$  \hspace{1cm} (4.58)

The values of the derivatives (4.57)–(4.58) are also used in the time step control algorithm. The scheme of the iterative solution is presented in Fig. 4.5.

### 4.4.5 Time step control

The time step size control poses substantial problem in the solution of highly nonlinear problems. There are two main factors that influence the time step size, namely the convergence of the nonlinear solver and the required accuracy of the solution. Usually the solution process begins with a small time step, especially if large gradients are imposed at the boundaries. The time step becomes larger as the solution varies slower from one time level to another.

One popular approach is to use an empirical algorithm based on the performance of the nonlinear solver (Simunek et al., 1998). The time step is adjusted in order to keep the number of iteration in each step in an "optimal" range, which is specified by the user. Although this method performs well for most typical problems, it can be ineffective for more difficult cases. In our case we used more rigorous algorithm (see Fig. 4.6), which is based on the estimation of the local truncation error introduced by the discretization in time (Tocci et al., 1997; Kavetski et al., 2001). For each time step we calculate the truncation error at each node $i$ as:

$$ \tau^{TR}_i = \left| \frac{\partial h}{\partial t} |^{j-1} \left| \frac{\partial h}{\partial t} |^j \right| \frac{\Delta t^{j-1}}{2} \right| $$  \hspace{1cm} (4.59)

and the maximum allowable error as:

$$ \tau^{ALL}_i = \tau^{ABS} + \tau^{REL} |h_i| $$  \hspace{1cm} (4.60)
where \( \tau^{\text{ABS}} \) and \( \tau^{\text{REL}} \) — user specified values of absolute and relative tolerance. If the condition:

\[
\tau_i^{TR} \leq s_1 \tau_i^{ALL}
\]  
(4.61)

is satisfied the time step is accepted and next step is taken. In (4.61) \( s_1 \) is a user specified safety parameter (for example \( s_1 = 0.9 \)). Otherwise the time step is repeated with the value of \( \Delta t \) reduced by a user specified multiplier \( f_1 \):

\[
\Delta t^j = f_1 \Delta t^j
\]  
(4.62)
The time step is also repeated if the nonlinear solver did not reach convergence in specified number of iterations $N_{ITMAX}$. If the condition:

$$
\tau_i^{TR} \leq s_2 \tau_i^{ALL}
$$

(4.63)

is satisfied in each node the solution is continued with new time step. Here $s_2$ is a user specified parameter smaller than $s_1$. The time step is increased according to the following formula:

$$
\Delta t^{i+1} = f_2 \Delta t^i
$$

(4.64)

increased by a user specified factor $f_2$ (for example 1.25). Moreover, the maximum and minimum allowable time step size ( $\Delta t_{max}$ and $\Delta t_{min}$ ) should be specified by the user as well as the initial step size ($t_{init}$). This type of time control algorithm ensures that $\Delta t$ varies according to the variation in the solution $h$. 


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Figure 4.6: Adaptive time stepping algorithm.
4.4.6 Solution of the linear tridiagonal systems

In each iteration a system of \( N \) linear equations (4.51) has to be solved to find the \( \Delta h \) increment. The system has tridiagonal matrix of coefficients. Due to this fact, it can be effectively solved by a direct method. In this case the Thomas method (Fletcher, 1991) was used, which is a variant of the lower-upper decomposition. The coefficients of jacobian matrix are stored in 3 one-dimensional arrays \( d, l \) and \( u \) and the right-hand side vector is denoted \( b = -f \). The array \( d \) represents the main diagonal, \( l \) — the lower diagonal and \( u \) — the upper diagonal. The algorithm is as follows:

1. Decomposition of the matrix
   \[
   d_i^* = d_i \\
   l_i^* = l_i/d_{i-1}^* \\
   d_i^* = d_i - l_i^* u_{i-1} \quad i = 2, \ldots, N
   \]

2. Modification of the right-hand side vector
   \[
   b_1^* = b_1 \\
   b_i^* = b_i - l_i b_{i-1}^* \quad i = 2, \ldots, N
   \]

3. Back-substitution
   \[
   \Delta h_N = b_N^*/d_N^* \\
   \Delta h_i = (b_i^* - u_i \Delta h_{i+1})/d_i^* \quad i = N - 1, \ldots, 1
   \]

4.5 Solution of the local flow equation

The local flow equation (3.55)–(3.56) is solved when the non-equilibrium flow is simulated (\( Q \neq 0 \) in equation (4.35). This problem has more simple form than the macroscopic one. The gravity term does not appear and the boundary condition is specified in terms of pressure head — constant over the boundary surface, but variable in time. Let us rewrite the local-scale flow equation in terms of dimensional variables:

\[
\frac{\partial \theta_2}{\partial t} - \frac{\partial}{\partial Y_i} \left( K_2 \frac{\partial h_2}{\partial Y_j} \right) = 0 \quad \text{in } \Omega_2 \tag{4.65}
\]

\[
h_2(\mathbf{X}, \mathbf{Y}, t) = h(\mathbf{X}, t) \quad \text{on } \Gamma \tag{4.66}
\]

where \( \mathbf{Y} \) is a dimensional local space variable. For the considered types of geometry one can take the advantage of the symmetry of the flow, thus reducing the size of the numerical
grid. The solution of (4.65) gives the local distribution of the water pressure head \( h_2 \) and the water content \( \theta_2 \) in inclusions. The source term in (4.35) is then calculated as:

\[
Q = \frac{1}{|\Omega|} \int_{\Omega_2} \theta_j^{i+1} - \int_{\Omega_2} \theta_j^i \Delta t
\]

where \( j \) is the time level index. The integrals in (4.67) are calculated numerically. The solution of the one-dimensional problems is performed with the same numerical procedure as the macroscopic equation, whereas the two- and three-dimensional equations are solved by spatial decomposition method, leading to a series of one-dimensional problems.

### 4.5.1 One-dimensional problems

One dimensional equation in orthogonal coordinates is used to simulate local flow for the slab-like geometry (geometry I, Fig. 4.2). It has the following form:

\[
\frac{\partial \theta_2}{\partial t} - \frac{\partial}{\partial Y_1} \left( K_2 \frac{\partial h_2}{\partial Y_1} \right) = 0 \quad (4.68)
\]

The equation (4.68) is solved in the domain \( 0 \leq Y_1 \leq a/2 \), where \( a \) is the width of the weakly conductive slab.

For the inclusions in form of cylinders (geometry III, Fig. 4.2) the problem can be transformed from the cartesian coordinates \((y_1, y_2)\) to the radial coordinates \((R, \varphi)\). Note that due to the symmetry the derivatives with respect to \( \varphi \) are equal to zero. Thus one obtains:

\[
\frac{\partial \theta_2}{\partial t} - \frac{\partial}{\partial r} \left( K_2 \frac{\partial h_2}{\partial r} \right) - \frac{1}{r} \left( K_2 \frac{\partial h_2}{\partial r} \right) = 0 \quad (4.69)
\]

which is solved in the domain \( 0 \leq r \leq R \) where \( R \) is the cylinder radius.

In order to simulate flow in the spherical inclusions (geometry V and VII, Fig. 4.2) the equation is transformed to the spherical coordinates \((r, \varphi, \psi)\). The derivatives with respect to \( \varphi \) and \( \psi \) being equal to zero, the following equation is obtained:

\[
\frac{\partial \theta_2}{\partial t} - \frac{\partial}{\partial r} \left( K_2 \frac{\partial h_2}{\partial r} \right) - \frac{2}{r} \left( K_2 \frac{\partial h_2}{\partial r} \right) = 0 \quad (4.70)
\]

The equations (4.68)–(4.70) are solved by an algorithm similar to the one used for the macroscopic problem. The equation is discretized with the finite differences (with constant \( \Delta Y \) or \( \Delta r \)). The Picard iterative method was used instead of the Newton scheme, since it requires less computational effort and proves efficient in this case.

The imposed boundary conditions reflects the symmetry of the flow:

- at the interface \( \Gamma \) the macroscopic pressure head is imposed — \( h_2 = h(X, t) \);
- in the center of the slab, circle or sphere the no-flux condition is applied — \( q = 0 \).
4.5.2 Two and three-dimensional problems

Two-dimensional problems arise for geometry II and IV (Fig. 4.2) and three-dimensional problems for geometry VI and VIII (Fig. 4.2). They can be written as:

\[
\frac{\partial \theta}{\partial t} - \left[ \frac{\partial}{\partial Y_1} \left( K_2 \frac{\partial h}{\partial Y_1} \right) + \frac{\partial}{\partial Y_3} \left( K_2 \frac{\partial h}{\partial Y_3} \right) \right] = 0 \tag{4.71}
\]

and:

\[
\frac{\partial \theta}{\partial t} - \left[ \frac{\partial}{\partial Y_1} \left( K_2 \frac{\partial h}{\partial Y_1} \right) + \frac{\partial}{\partial Y_2} \left( K_2 \frac{\partial h}{\partial Y_2} \right) + \frac{\partial}{\partial Y_3} \left( K_2 \frac{\partial h}{\partial Y_3} \right) \right] = 0 \tag{4.72}
\]

respectively. Since the numerical solution of two- and three-dimensional nonlinear flow equations can be tedious and time consuming, the fractional step method was used. It allows splitting the solution of a two- or three-dimensional problem into a series of one dimensional problems at each time step (Quarteroni & Valli, 1997; Daus & Frind, 1985; Nawalany, 1991).

For the two-dimensional flow, the solution is divided into 2 sub-steps.

1. Solution in the $Y_1$ direction with the initial condition $h^{(0)}$, which gives the first intermediate value $h^{(1/2)}$:

\[
\frac{\theta^{i+1/2}}{\Delta t} - \frac{\theta^{i}}{\Delta t} = \left[ \xi L_1^{i+1/2} + (1 - \xi) L_1^i \right] \tag{4.73}
\]

where the spatial operator $L_1$ denotes:

\[
L_1 = \frac{1}{\Delta Y_1} \left[ K_{i+1/2} \frac{h_{i+1,\kappa} - h_{i,\kappa}}{\Delta Y_1} - K_{i-1/2} \frac{h_{i,\kappa} - h_{i-1,\kappa}}{\Delta Y_1} \right] \tag{4.74}
\]

and the indices $i$ and $\kappa$ refer to the position of the node in the $Y_1$ and $Y_3$ direction respectively.

2. Solution in $Y_2$ direction with the initial condition $h^{(1/2)}$, which gives the final value $h^{(1)}$:

\[
\frac{\theta^{i+1}}{\Delta t} - \frac{\theta^{i+1/2}}{\Delta t} = \left[ \xi L_2^{i+1} + (1 - \xi) L_2^{i+1/2} \right] \tag{4.75}
\]

where the spatial operator $L_3$ denotes:

\[
L_3 = \frac{1}{\Delta Y_3} \left[ K_{\kappa+1/2} \frac{h_{i,\kappa+1} - h_{i,\kappa}}{\Delta Y_3} - K_{\kappa-1/2} \frac{h_{i,\kappa} - h_{i,\kappa-1}}{\Delta Y_3} \right] \tag{4.76}
\]

For three-dimensional geometry three sub-steps arise at each time step:

1. Solution in the $Y_1$ direction with the initial condition $h^{(0)}$, which gives the first intermediate value $h^{(1/3)}$:

\[
\frac{\theta^{i+1/3}}{\Delta t} - \frac{\theta^{i}}{\Delta t} = \left[ \xi L_1^{i+1/3} + (1 - \xi) L_1^i \right] \tag{4.77}
\]
where the spatial operator \( \mathcal{L}_1 \) denotes:

\[
\mathcal{L}_1 = \frac{1}{\Delta Y_1} \left[ K_{i+1/2} \frac{h_{i+1,\kappa,\lambda} - h_{i,\kappa,\lambda}}{\Delta Y_1} - K_{i-1/2} \frac{h_{i,\kappa,\lambda} - h_{i-1,\kappa,\lambda}}{\Delta Y_1} \right] \tag{4.78}
\]

and the indices \( \iota, \kappa, \lambda \) refer to the position of node in the \( Y_1, Y_2 \) and \( Y_3 \) direction respectively.

2. Solution in the \( Y_2 \) direction with the initial condition \( h^{(1/3)} \), which gives the second intermediate value \( h^{(2/3)} \).

\[
\frac{\theta_{i}^{j+2/3} - \theta_{i}^{j+1/3}}{\Delta t} - \left[ \xi \mathcal{L}_2^{j+2/3} + (1 - \xi) \mathcal{L}_2^{j+1/3} \right] = 0 \tag{4.79}
\]

where the spatial operator \( \mathcal{L}_2 \) denotes:

\[
\mathcal{L}_2 = \frac{1}{\Delta Y_2} \left[ K_{\kappa+1/2} \frac{h_{i,\kappa+1,\lambda} - h_{i,\kappa,\lambda}}{\Delta Y_2} - K_{\kappa-1/2} \frac{h_{i,\kappa,\lambda} - h_{i,\kappa-1,\lambda}}{\Delta Y_2} \right] \tag{4.80}
\]

3. Solution in the \( Y_3 \) direction with the initial condition \( h^{(2/3)} \), which gives the final value \( h^{(1)} \).

\[
\frac{\theta_{i}^{j+1} - \theta_{i}^{j+2/3}}{\Delta t} - \left[ \xi \mathcal{L}_3^{j+1} + (1 - \xi) \mathcal{L}_3^{j+2/3} \right] = 0 \tag{4.81}
\]

where the spatial operator \( \mathcal{L}_3 \) denotes:

\[
\mathcal{L}_3 = \frac{1}{\Delta Y_3} \left[ K_{\lambda+1/2} \frac{h_{i,\kappa,\lambda+1} - h_{i,\kappa,\lambda}}{\Delta Y_3} - K_{\lambda-1/2} \frac{h_{i,\kappa,\lambda} - h_{i,\kappa,\lambda-1}}{\Delta Y_3} \right] \tag{4.82}
\]

In each sub-step a series of one-dimensional problems arises, which are solved by the algorithm described before. Note that in order to reduce the error resulting from decomposition of the equation the value of time weighting parameter \( \xi \) should be close to 0.5 (Quarteroni & Valli, 1997; Le Pourhiet, 1988).

Due to the symmetry the equations are solved in a quarter of the rectangle or one-eights of the block respectively. At the edges or surfaces corresponding to the interface \( \Gamma \) the macroscopic pressure head is imposed, while the inner surfaces are treated as no-flux boundaries.

### 4.6 Code DPOR–1D

The DPOR–1D code was written in Fortran 90 programming language and was run on machines with Windows 2000/XP and Unix operating systems. The general scheme of the code is presented in Fig. 4.7, the users manual can be found in Appendix A and the listing in Appendix B.
Figure 4.7: General scheme of the DPOR–1D code. Dashed lines indicates the part which is executed only for the local non-equilibrium flow model. Names of the procedures are printed in italics.
4.6.1 Tests

A number of numerical tests have been performed, aimed at the evaluation of the performance of the code.

First, the solution of the local boundary value problems were compared to the analytical solution available for the geometry I and II (Fig. 4.2) and to the results obtained from MONO3D code (Quintard, 1997) and from FEMLAB commercial software for other types of geometry. Generally, a good agreement of the results was obtained. Nevertheless the tests revealed some limitations of the code. Since the whole period domain is discretized, the number of nodes is much greater than it would be when the numerical grid comprised one sub-domain only. On the other hand the grid size influences the results. Finer discretization is required for spherical and cylindrical inclusions and when the volume fraction of inclusions tends to 1.

Other tests included comparison of the macroscopic flow model for the equilibrium case with the Philip semi-analytical solution and numerical solutions from HYDRUS-1D (Šimůnek et al., 1998) and UNSAT-H (Fayer, 2000) programs. Finally the solution of three-dimensional flow in cubic aggregates was compared to the analytical solution available for linear flow. In all those cases the results of DPOR-1D simulations were close to the reference analytical solutions. Although the comparisons concerned relatively simple situations (equilibrium flow), one can expect that the code performs well also in more complicated non-equilibrium cases.

Another series of tests concerned the solution of macroscopic flow equation for various initial and boundary conditions. Both local non-equilibrium and local equilibrium flow problems were solved. As it could be expected the solution of the local non-equilibrium model with coupled macroscopic and local variables is much more time-consuming than in the case of equilibrium-type Richards equation. This is due to the source term, which requires solution of the local-scale flow equation at each node. When the local flow equations are one dimensional, the simulation time is about 5 to 10 times longer for the local non-equilibrium case. For two- and three-dimensional cases the time increases further by two or three orders of magnitude. On the other hand, the solution still requires less effort and time, than the direct simulation in heterogenous domain (fine scale solution). Thus, from practical point of view it would be convenient to simplify the calculation of source term by introducing some closed form analytical formula. Note that such formulas are available in the literature, but their applicability for highly transient unsaturated flow might be questionable. Alternatively one can consider replacing two- and three-dimensional problems by an equivalent one-dimensional formulation. When the local problems are one-dimensional the solution is still possible within a reasonable time. This problem would be important in view of the possible extension of the
code for macroscopically two-dimensional flow or the application to the inverse problems.

An important question in the solution of highly nonlinear problems is the stability of the solution and the convergence of the nonlinear solver. Our tests showed that they are related to the initial and boundary conditions and the hydraulic characteristics of the two porous materials. Generally, the code performed well for a wide range of conditions, and only occasional problems with convergence were encountered. In such case adjustment of the numerical parameters was necessary. A detailed analysis of the influence of various numerical parameters on the performance of the program is beyond the scope of this study.

Some examples of the calculation of the effective parameters are presented in Chapter 5, while in Chapter 6 we discuss in the solutions of three macroscopic problems in more detailed way.

4.6.2 Conclusions

The tests performed with DPOR–1D code allow to formulate some preliminary conclusions concerning the following issues:

1. The numerical experiments showed, that the choice of the weighting parameter $\xi$ has relatively little influence on the solution. The fully implicit scheme $\xi = 1$ ensured the best convergence of the nonlinear solver. For smaller values the mass balance was slightly better, but the number of iterations increased. The value of $\xi$ should not be less than 0.55. For $\xi = 0.5$ the solution was occasionally unstable.

2. The linearization of the source term with respect to $h$ according to the formula (4.51) significantly reduces the time of calculation in some cases. However this approach is not universal, since for some more difficult sets of hydraulic functions and boundary conditions the iterative process fails to converge. In such cases it is recommended to solve the local-scale flow equations in each iteration and update the source term consecutively.

3. The solution process is significantly influenced by the required accuracy and the time step control parameters. The proposed algorithm, based on the estimation of the truncation error generally requires more time steps compared to the routinely used algorithms based on the performance of the iterative solver. Nevertheless, it proved to be more efficient, in terms of the stability of the solution. On the other hand, in some cases it is necessary to force the code not to reduce the time step and to proceed with the solution, even if the accuracy criterion is not met. This can be done by the proper choice of the control parameters ($f_1 = 1$).
The program in its present form offers room for further improvements. They may include: introduction of additional types of the local geometry (e.g. ellipsoidal inclusions), implementation of the local equilibrium flow model for the moderately heterogenous soils with the corresponding local boundary value problem (Lewandowska & Laurent, 2001), simplified formulations of the exchange term in the non-equilibrium model, other models of hydraulic functions with possible tabularization and interpolation, non-uniform spatial discretization, or the user interface.
Chapter 5

Effective conductivity of the double-porosity soils

5.1 Introduction

The method of homogenization enables us to derive the effective properties characterizing the behavior of a heterogeneous medium at the macroscopic scale. The two effective parameters appearing in the macroscopic models developed in Chapter 3 are the effective capillary capacity $C_{\text{eff}}$ and the effective hydraulic conductivity $K_{\text{eff}}$. They are the intrinsic parameters of the medium, independent of the macroscopic initial and boundary conditions. They are estimated from local hydraulic properties of the two regions and require information on the structural geometry of the medium. The calculation of the effective capillary capacity is straightforward since it requires only the volume fraction of the two sub-domains. The effective conductivity, in contrast, is obtained from the solution of the local boundary value problem, which in most cases has to be performed numerically.

In Chapter 3 it has been shown that we have three different formulations of the local boundary value problem according to the ratio of the hydraulic conductivity of the two components of the double-porosity medium. Let us briefly recall the corresponding problems (for simplicity we assume that both sub-domains are locally isotropic):

1. For moderately heterogeneous media (Lewandowska & Laurent, 2001) one obtains the
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problem defined over the entire period volume Ω:
\[
\frac{\partial}{\partial y_i} \left[ K^{(0)}_1 \left( I_{ik} + \frac{\partial \chi^I_k}{\partial y_i} \right) \right] = 0 \quad \text{in } \Omega_1 \tag{5.1}
\]
\[
\frac{\partial}{\partial y_i} \left[ K^{(0)}_2 \left( I_{ik} + \frac{\partial \chi^{II}_k}{\partial y_i} \right) \right] = 0 \quad \text{in } \Omega_2 \tag{5.2}
\]
\[
\chi^I_i = \chi^{II}_i \quad \text{on } \Gamma \tag{5.3}
\]
\[
K^{(0)}_1 \left( I_{ik} + \frac{\partial \chi^I_k}{\partial y_i} \right) N_i = K^{(0)}_2 \left( I_{ik} + \frac{\partial \chi^{II}_k}{\partial y_i} \right) N_i \quad \text{on } \Gamma \tag{5.4}
\]
where \( \chi^I \) and \( \chi^{II} \) are \( y \)-periodic and \( \langle \chi \rangle = 0 \). \( K^{(0)}_{1ij} \) and \( K^{(0)}_{2ij} \) denote the local conductivities of the two components, and \( N \) is the unit vector normal to the interface \( \Gamma \). The effective conductivity is written:
\[
K_{ij}^{\text{eff}} (h^{(0)}) = \frac{1}{|\Omega|} \left( \int_{\Omega_1} K^{(0)}_1 \left( I_{ij} + \frac{\partial \chi^I_j}{\partial y_i} \right) d\Omega_1 + \int_{\Omega_2} K^{(0)}_2 \left( I_{ij} + \frac{\partial \chi^I_j}{\partial y_i} \right) d\Omega_2 \right) \tag{5.5}
\]

2. For the media with the inclusions much less conductive than the matrix the local problem is defined over the matrix part of the period \( \Omega_1 \), with Neuman-type condition at the interface \( \Gamma \):
\[
\frac{\partial}{\partial y_i} \left[ K^{(0)}_{1ij} \left( I_{jk} + \frac{\partial \chi^I_k}{\partial y_j} \right) \right] = 0 \quad \text{in } \Omega_1 \tag{5.6}
\]
\[
K^{(0)}_{1ij} \left( I_{jk} + \frac{\partial \chi^I_k}{\partial y_j} \right) N_i = 0 \quad \text{on } \Gamma \tag{5.7}
\]
where \( \chi \) is \( y \)-periodic \( \langle \chi \rangle = 0 \). In this case the effective conductivity is a linear function of the matrix conductivity, defined by the following formula:
\[
K_{ij}^{\text{eff}} (h^{(0)}) = \frac{K_1}{|\Omega|} \int_{\Omega_1} \left( I_{ij} + \frac{\partial \chi^I_j}{\partial y_i} \right) d\Omega_1 \tag{5.8}
\]

3. For the media with the inclusions much more conductive than the matrix the local problem is defined over the matrix part of the period \( \Omega_2 \), with a Dirichlet-type boundary condition on \( \Gamma \).
\[
\frac{\partial}{\partial y_i} \left[ K^{(0)}_{2ij} \left( I_{ik} - \frac{\partial \chi^I_k}{\partial y_j} \right) \right] = 0 \quad \text{in } \Omega_1 \tag{5.9}
\]
\[
\chi_k = y_k \quad \text{on } \Gamma \tag{5.10}
\]
and \( \chi \) is \( y \)-periodic. The components of the effective conductivity tensor are defined as:
\[
K_{ij}^{\text{eff}} (h^{(0)}) = \frac{K_2}{|\Lambda|} \int_{\Lambda} \left( I_{ij} - \frac{\partial \chi^I_j}{\partial y_i} \right) d\Lambda \tag{5.11}
\]
Similarly to the previous case, the effective conductivity is a linear function of the matrix conductivity.
Chapter 5. Effective conductivity of the double-porosity soils

One should note that the effective conductivity of highly heterogeneous soils calculated from (5.8) and (5.11) can be written in the form $K_{\text{eff}} = K_1 K_E$ where $K_E$ represents the integral term, which is constant for a given local geometry. In such case the local boundary problem should be solved only once. For moderately heterogeneous medium the definition of the effective conductivity involves the parameters of both components $K_1(h)$ and $K_2(h)$ and the local boundary value problem needs to be solved for each value of the macroscopic pressure head $h$.

As it has been pointed out in Chapter 3, the second and third type of problem can be regarded as the limit cases of the first problem. In (5.6)–(5.7) the inclusions are considered effectively impermeable, while in (5.9)–(5.10) they are treated as infinitely permeable. Similar mathematical formulations have been developed by other authors studying flow in porous media either by homogenization method (Arbogast et al., 1990; Hornung, 1991; Panfilov et al., 1997) or by the volume averaging method (Quintard & Whitaker, 1988).

The presented results can also be considered in a more general context of estimating the effective transfer properties in heterogeneous media. This issue has been addressed in numerous publications from the field of groundwater and petroleum engineering (Wen & Gómez-Hernández, 1996; Renard & de Marsily, 1997). One should also note the contributions concerning heat transfer, electric conductivity or diffusion (Clyne, 2000; Aramyan & Karapetyan, 2001; Mei et al., 1997; Auriault, 1983), which are physical processes governed by similar mathematical equations.

In the following sections we examine some factors influencing the effective conductivity of a double-porosity medium. These factors are: (i) the ratio of the conductivities of the two sub-domains, (ii) the volumetric fraction of inclusions, (iii) the spatial arrangement of the inclusions and (iv) the anisotropy of the medium. The numerical results are compared with theoretical bounds of Wiener (1912) and Hashin & Shtrikman (1962).

Finally, it should be pointed out that the problems (5.1)–(5.4), (5.6)–(5.7) and (5.9)–(5.10) defining the effective conductivity reflect different flow conditions and are closely associated with the respective macroscopic models.

5.2 Upper and lower bounds for the effective conductivity

According to the analysis by homogenization the effective conductivity of a double-porosity medium depends in a general case on the following factors: the local conductivities $K_1$ and $K_2$, the volume fractions of the sub-domains $w_1$ and $w_2$ and the geometry of the medium. For the same values of $K_1$, $K_2$, $w_1$ and $w_2$ but different spatial arrangements of the $\Omega_1$ and
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$\Omega_2$ sub-domains quite different values of $K^{eff}$ will result.

The effective conductivity obtained from homogenization can be compared with the classical lower and upper bounds developed for mixtures by Wiener (1912) and Hashin & Shtrikman (1962). These bounds are functions of the conductivity of each constituent and their volume fractions. They concern saturated conditions.

The following relation for the effective conductivity is usually attributed to Wiener (1912):

$$K^{har} \leq K^{eff} \leq K^{ar}$$

(5.12)

where $K^{har}$ and $K^{ar}$ denotes respectively the harmonic mean and the arithmetic mean of the constituents conductivities:

$$K^{har} = \frac{K_1K_2}{w_1K_2 + w_2K_1}$$

(5.13)

$$K^{ar} = w_1K_1 + w_2K_2$$

(5.14)

Since the relation (5.12) is always satisfied, $K^{ar}$ and $K^{har}$ are also called fundamental bounds. They correspond to the classical results obtained for flow (and other transport processes) in stratified systems.

Hashin & Shtrikman (1962) proposed the following bounds for isotropic bi-component medium:

$$K^{ar} - \frac{w_1w_2(K_1 - K_2)^2}{(D - w_2)K_2 + w_2K_1} \leq K^{eff} \leq K^{ar} - \frac{w_1w_2(K_1 - K_2)^2}{(D - w_1)K_1 + w_1K_2}$$

(5.15)

where $D$ is the dimension of the problem ($D = 2$ for two-dimensional geometries and $D = 3$ for three-dimensional geometries). The Hashin–Shtrikman bounds were obtained for a model medium made of composite spheres of variable diameter. Each sphere consists of a kernel surrounded by an envelope of different conductivity. The lower bound corresponds to the situation when spheres of low conductivity $K_2$ are embedded in highly conductive envelopes $K_1$. The upper bound represents inverse case, i.e. highly conductive spheres in weakly conductive shells.

When the two components have contrasting conductivities, both Wiener and Hashin-Shtrikman bounds give relatively large range of variability of $K^{eff}$. Fig. 5.1 presents the bounds for a binary medium as function of the volume fraction of the more conductive material. The values were calculated assuming that $K_1 = 1$ and $K_2 = 0.0001$. The widest range is given by Wiener bounds. Note also that the values of Hashin-Shtrikman bounds are slightly larger for three-dimensional geometries compared to two-dimensional. Other bounds are also available in the literature, including Cardwell & Parsons (1945); Ene (1991); Matheron (1968, 1993). In the following sections we use the Wiener and Hashin-Shtrikman bounds for comparison purposes.
5.3 Study of the limit passages between local boundary value problems

In order to study the limit passage between the local boundary value problem (5.1)–(5.4) and the problems (5.6)–(5.7) and (5.9)–(5.10) a series of numerical calculations using the MONO3D program (Quintard, 1997) was performed. The local problem (5.1)–(5.4) was solved for two types of local geometry: two-dimensional geometry with square inclusion (Fig. 5.2b) and three-dimensional geometry with cubic inclusion (Fig. 5.2d). The inclusions are placed centrally in a period of unit volume. The volume fractions of inclusions are 0.49 for two-dimensional geometry and 0.512 for three-dimensional geometry. The calculations were performed for the two possible cases, i.e. inclusions less conductive and more conductive than the matrix. In each case the ratio of conductivity of the matrix $K_{\text{mat}}$ to the conductivity of the inclusions $K_{\text{inc}}$ was varied from $\frac{K_{\text{inc}}}{K_{\text{mat}}} = 10^{-6}$ to $\frac{K_{\text{inc}}}{K_{\text{mat}}} = 10^{6}$. A fine spatial discretization was used: $100 \times 100$ gridblocks for 2D problem and $100 \times 100 \times 100$ gridblocks for 3D problem. In each case the effective conductivity was calculated from the definition (5.5). The obtained results are presented in Fig. 5.3. The ratio of effective conductivity to the conductivity of the matrix $\frac{K_{\text{eff}}}{K_{\text{matrix}}}$ is plotted as function of $\frac{K_{\text{inc}}}{K_{\text{mat}}}$ ratio. We can see the asymptotic behavior.
of $K^{eff}$ when the contrast of the parameters increases. For two-dimensional inclusions the effective conductivity tends to constant values $K^{eff} = 0.33 \, K_{mat}$ for $\frac{K_{inc}}{K_{mat}} \ll 10^{-2}$ and $K^{eff} = 3.01 \, K_{mat}$ for $\frac{K_{inc}}{K_{mat}} \gg 10^3$. For three-dimensional inclusions the limit values $K^{eff} = 0.38 \, K_{mat}$ and $K^{eff} = 4.48 \, K_{mat}$ are reached for $\frac{K_{inc}}{K_{mat}} \ll 10^{-2}$ and $\frac{K_{inc}}{K_{mat}} \gg 10^3$ respectively. Those values of $K^{eff}$ correspond to the values obtained from the solution of (5.6)–(5.7) and (5.9)–(5.10). Thus it can be concluded that the problem (5.6)–(5.7) can be regarded as the limiting case of the problem (5.1)–(5.4) when $\frac{K_{inc}}{K_{mat}}$ tends to 0, while the problem (5.9)–(5.10) is a limiting case of the problem (5.1)–(5.4) when $\frac{K_{inc}}{K_{mat}}$ tends to infinity.

### 5.4 Effective conductivity as a function of the water pressure head

In the soils with inclusions much less conductive or much more conductive than the matrix the effective conductivity $K^{eff}$ is a linear function of the matrix conductivity $K_{mat}$. The ratio $\frac{K^{eff}}{K_{mat}}$ depends on the geometry of the period and is given by the integral of function in (5.8) and (5.11). Since the matrix conductivity depends on the water pressure head $h$, the effective conductivity is a function of $h$ as well. The relation is highly nonlinear and...
depends on the characteristics of the interconnected matrix. As an example we calculated the effective conductivity functions for a soil with inclusions in the form of squares (Fig. 5.2b). We considered two cases: (i) inclusions less conductive than the matrix and (ii) inclusions more conductive than the matrix.

In the first case the matrix characteristics correspond to loamy sand (according to Carsel & Parrish (1988)). The hydraulic conductivity is given by the Mualem – van Genuchten formula:

$$K = K_s \frac{\left[1 - (\alpha|h|)^{n-1} \left[1 + (\alpha|h|)^n\right]^{-m} \right]^2}{\left[1 + (\alpha|h|)^{n} \right]^{m/2}}$$

with the following parameters: $K_s = 14.59 \text{ cm h}^{-1}$, $\alpha = 0.124 \text{ cm}^{-1}$, $n = 2.280$, $m = 1 - 1/n = 0.561$. It is assumed that the relation $K_{\text{mat}}(h) \gg K_{\text{inc}}(h)$ is satisfied in the whole range of the water pressure head. The effective conductivity curves for different volume fractions of inclusions are presented in Fig. 5.4a. Note that the shape of the curve remains the same, whereas the values of $K^{\text{eff}}$ decrease as the volume fraction of inclusions increase.

In the second case we assumed that the weakly conductive matrix has typical silty clay
parameters (Carsel & Parrish, 1988): \( K_s = 0.02 \, \text{cm h}^{-1}, \alpha = 0.005 \, \text{cm}^{-1}, n = 1.090, m = 1 - 1/n = 0.826 \). The \( K_{eff}(h) \) curves obtained for different volume fractions of inclusions are presented in Fig. 5.4b. As in previous case, the effective functions corresponds to the \( K_{mat}(h) \) curve scaled by a factor resulting from the geometry.

One should note that in general case the ratio of hydraulic conductivities of the two components varies as a function of the water pressure head. In dry conditions (high absolute values of \( h \)) clayey soils are more conductive than sandy soils, whereas in wet conditions the situation is inverse. Thus, for a composite soil made of sand and clay the \( K(h) \) curves can be crossed. In order to illustrate this problem numerical calculations were performed for two types of soil: (i) loamy sand matrix with silty clay inclusions and (ii) silty clay matrix with loamy sand inclusions. We used the same geometry as in previous examples and we assumed that the volume fraction of inclusions is (i) \( w_2 = 0.49 \) and (ii) \( w_1 = 0.49 \), respectively. In each case the effective conductivity was calculated from the solution of the local boundary problem (5.6)–(5.7). The solution was obtained using MONO-3D code (Quintard, 1997). We also calculated \( K_{eff} \) from the problems (5.6)–(5.7) and (5.9)–(5.10), respectively, using the DPOR-1D code. The two latter formulations result from the estimation of ratio for the wet domain (\(|h| < 10 \, \text{cm}\)). The results are shown in Figs 5.5a and 5.5b. Note that the effective conductivity curves coincide in the wet range, i.e. when the estimation holds. In the dry range a discrepancy exists between the two formulations. This is due to the fact that the
conductivity curves of the two components are crossed.

At this point we should emphasize the fact that the effective conductivity is closely related to the corresponding macroscopic model. The choice of adequate macroscopic model results from the flow conditions. Different models are appropriate for the flow in wet and dry domain.

5.5 Influence of the volume fraction of inclusions

In this section we analyze the behavior of the effective conductivity in the double-porosity medium as a function of the volume fraction of inclusions. We consider four particular types of geometry (Fig. 5.2a-d):

- two-dimensional inclusions: circles and squares,
- three-dimensional inclusions: spheres and cubes.

For each geometry two series of numerical calculations were performed using the DPOR-1D code: (i) the inclusions much less conductive than the matrix and (ii) the inclusions much more conductive than the matrix. The period of unit volume was discretized with a uniform grid of $101 \times 101 \times 101$ nodes. Due to the symmetry properties the effective conductivity reduces to a scalar: $K^\text{eff} = K^\text{eff} \mathbf{I}$, where $\mathbf{I}$ is identity matrix.
Figure 5.6: Solution of the local boundary value problem for weakly conductive square inclusions, \( w_2 = 0.49 \): (a) – function \( \chi_3 \) and (b) – its gradient \( \left[ 1 + \frac{\partial \chi_3}{\partial y_3} \right] \).

Figure 5.7: Solution of the local boundary value problem for highly conductive square inclusions, \( w_1 = 0.49 \): (a) – function \( \chi_3 \) and (b) – its gradient \( \left[ 1 - \frac{\partial \chi_3}{\partial y_3} \right] \).
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For all calculations we assumed that the ratio of the conductivity of the highly conductive \((K_1)\) sub-domain and the weakly conductive \((K_2)\) sub-domain is: \(\frac{K_2}{K_1} = 10^{-4}\). In the first series the effective conductivity is defined by the problem (5.6)–(5.7). As an example of the solution in Fig. 5.6 we show the function \(\chi_3\) and its gradient \(1 + \frac{\partial \chi_3}{\partial y_3}\) obtained for a square inclusion (Fig. 5.2)b, volume fraction of inclusion \(w_2 = 0.49\). Note the symmetry and the periodicity of \(\chi_3\). Since the effective conductivity is a linear function of the conductivity of the highly conductive matrix, the results can be conveniently presented as the relation between \(\frac{K^{\text{eff}}}{K_1}\) ratio and the volume fraction of inclusions \(w_2\), where \(w_2\) varies from 0 to 1. Fig. 5.8a shows this relation for two-dimensional geometries. The results are compared with the theoretical bounds of Wiener and Hashin-Shtrikman. Note that the lower bounds are very close to zero. The values of \(K^{\text{eff}}\) obtained from homogenization coincide with the Hashin-Shtrikman upper bound. The difference between circles and squares is not significant. When the diameter of circle is equal to the period length \((w_2 = 0.785)\) the effective conductivity is \(K^{\text{eff}} = 0\) because the circles are touching each other and the flow is not possible.

Similar results were obtained for three-dimensional geometries, Fig. 5.8b. Note that the calculations for spherical inclusions were extended for the case when the diameter of the sphere is greater than 1. It corresponds to the situation when the neighboring inclusions are partially overlapping and the weakly conductive sub-domain is continuous. Nevertheless, the results show the same tendency as when the spheres are not connected. The values of \(K^{\text{eff}}\) for two-dimensional inclusions are slightly smaller than for 3D inclusions for the same
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Figure 5.9: Effective conductivity of the double-porosity medium with highly conductive inclusions: (a) – 2D inclusions, (b) – 3D inclusions.

The second series of calculations was performed for inclusions more conductive than the matrix. We assumed the same parameter ratio, i.e. $\frac{K_2}{K_1} = 10^{-4}$. An example of the solution of the local problem (5.9)–(5.10) is shown in Fig. 5.7. The solution was obtained for a two-dimensional square inclusion, the volume fraction of inclusion being $w_1 = 0.49$. The calculated values of $K^{eff}$ as function of the volume fraction of inclusions $w_1$ are presented in Fig. 5.9a (2D geometries) and in Fig. 5.9b (3D geometries). Note that the effective conductivity obtained from the solution of the local problem (5.9)–(5.10) tends to infinity, when the volume fraction of inclusions $w_1$ approaches 1. At the same time the lower bounds of Wiener and Hashin-Shtrikman, which are calculated for finite values of $K_1$ and $K_2$ tend to the value $K_1$. Similarly to the previous case, the differences between spheres and cubes and between circles and squares are negligible. Again, the effective conductivity for the same $w_1$ is larger for a three-dimensional geometry than for a two-dimensional geometry. The results coincide with the lower bound of Hashin and Shtrikman.

5.6 Influence of the spatial arrangement of inclusions

In this section we examine the influence of the spatial arrangement of inclusions on the effective conductivity. We consider a medium with weakly conductive inclusions in form of spheres and cubes. We assume that the inclusions may touch each other, but cannot be
connected. Three types of packing are examined (Fig. 5.10):

- **Case A**: *simple cubic* geometry (SC) (Fig. 5.10a), where the inclusions of uniform size are placed in the corners of a unit size cubic period; for the spheres the maximum possible radius is \( R_{\text{max}} = 0.5 \), which corresponds to the volumetric fraction of spheres \( w_2 = 0.524 \); for the cubes the edge length \( a \) may vary between 0 and 1; this geometry is equivalent to a single inclusion placed in the center of the cube (Fig. 5.2b);

- **Case B**: *centered cubic* geometry (CC) (Fig. 5.10b), where the inclusions are placed in the corners and in the center of a cubic period; in this case maximum possible sphere radius is \( R_{\text{max}} = 0.433 \), which corresponds to \( w_2 = 0.64 \); for the cubic inclusions the maximum dimension is \( a_{\text{max}} = 0.25 \), which gives volume fraction \( w_2 = 0.125 \);

- **Case C**: *centered parallelepiped* geometry (CP) (Fig. 5.10c), where the inclusions are placed in the corners and in the center of paralelepiped period; for spherical inclusions the dimensions of the period are: \( 1 \times 1 \times \sqrt{2} \). For the radius \( R_{\text{max}} = 0.5 \) one obtains \( w_2 = 0.74 \) which is the maximum possible volume fraction of spheres; for cubic inclusions the dimensions are: \( 1 \times 1 \times 2 \) and the cube length varies from 0 to 1.

The solutions were obtained with the code DPOR-1D. A uniform discretization was used: \( 101 \times 101 \times 101 \) nodes for Cases A and B, \( 101 \times 101 \times 141 \) for Case C with spherical inclusions and \( 101 \times 101 \times 201 \) for Case C with cubic inclusions. The results of the calculation of the effective conductivity for different arrangements of inclusions are presented in Fig. 5.11a (spheres) and in Fig. 5.11b (cubes). In this figures we present the values of \( K_{33}^{\text{eff}} \) component of the effective conductivity tensor. Note that due to the symmetry properties we obtained \( K_{11}^{\text{eff}} = K_{22}^{\text{eff}} = K_{33}^{\text{eff}} \) for SC and CC geometry.

As it can be seen, the values corresponding to the same fraction of inclusions are nearly the same for different arrangements. Thus it can be concluded, that for the simple geometry of inclusions considered the effective conductivity depends mainly on the volume fraction of spheres or cubes.

### 5.7 Anisotropy of the effective conductivity tensor

In order to capture the effect of anisotropy on the effective conductivity tensor, numerical calculations were performed for two-dimensional rectangular inclusions shown in Fig. 5.2e. The period is a square of unit dimensions. The inclusion is placed centrally. The volume of inclusion is set to 0.16, while its shape is varied. The shape is defined by the ratio of edge lengths \( \frac{a_1}{a_3} \), which varies in the range 1, \ldots, 6. Due to the symmetry the \( K^{\text{eff}} \) components
outside the main diagonal are equal to zero. As in the previous section, we analyzed the case with weakly conductive inclusions and the case with highly conductive inclusions. The calculations were performed using DPOR,1D code on uniform grid 201 × 201 nodes.

The relation between the aspect ratio $a_1/a_3$ and the effective conductivity in $y_1$ and $y_3$ direction for the soil with less conductive inclusions is presented in Fig. 5.12a and for the soil with more conductive inclusion in Fig. 5.12b. The effective conductivity in $y_1$ direction $K_{11}^{\text{eff}}$ is different from the conductivity in $y_3$ direction $K_{33}^{\text{eff}}$ when $a_1/a_3 > 1$. The calculated coefficients are compared with the Wiener bounds. It can be seen that for weakly conductive inclusions $K_{11}^{\text{eff}}$ approaches upper bound of Wiener, while for highly conductive inclusions $K_{33}^{\text{eff}}$ approaches the lower bound, when the ratio $a_1/a_3$ is increased. Note that for $a_1/a_3 = 6.25$ one obtains a stratified system, where the effective conductivity in the direction parallel and orthogonal to the layers is given by upper and lower Wiener bound respectively.

In Figs 5.13, 5.14, 5.15 and 5.16 we show examples of the calculated components of vector function $\chi_1$ and $\chi_3$ and their gradients, respectively. The solutions were obtained for the
Figure 5.11: Effective conductivity of the double-porosity medium with for different spatial arrangements of inclusions: (a) – spherical inclusions, (b) – cubic inclusions.

Figure 5.12: Effective conductivity of the double-porosity medium for anisotropic local geometry: (a) – weakly conductive inclusions, (b) – highly conductive inclusions.
Figure 5.13: Solution of the local boundary value problem for weakly conductive anisotropic inclusions, $\frac{a_1}{a_3} = 4$: (a) – function $\chi_1$ and (b) – its gradient $\left[1 + \frac{\partial \chi_1}{\partial y_1}\right]$.

Figure 5.14: Solution of the local boundary value problem for highly conductive square inclusions, $\frac{a_1}{a_3} = 4$: (a) – function $\chi_3$ and (b) – its gradient $\left[1 + \frac{\partial \chi_3}{\partial y_3}\right]$. 
Figure 5.15: Solution of the local boundary value problem for highly conductive anisotropic inclusions, \( a_1/a_3 = 4 \): (a) – function \( \chi_1 \) and (b) – its gradient \( [1 - \frac{\partial \chi_1}{\partial y_1}] \).

Figure 5.16: Solution of the local boundary value problem for highly conductive anisotropic inclusions, \( a_1/a_3 = 4 \): (a) – function \( \chi_3 \) and (b) – its gradient \( [1 - \frac{\partial \chi_3}{\partial y_3}] \).
aspect ratio $a_1/a_3 = 4$. One can see the patterns of the perturbation around the inclusion, corresponding to different flow directions. The figures can be compared with the isotropic cases (Figs 5.6 and 5.7).

## 5.8 Summary

Although the presented analysis is far from being exhaustive it enables us to draw some conclusions on the macroscopic parameters in double-porosity media.

It has been shown, that for large contrast of the constituents conductivity the effective conductivity is determined by the conductivity of the interconnected (matrix) region. Numerical calculations showed that the influence of the conductivity of inclusions may be neglected if $K_2/K_1$ is sufficiently small, $K_2/K_1 \ll 10^2$. It confirms the applicability of the local problems (5.6)–(5.7) and (5.9)–(5.10) as limit cases of the problem (5.1)–(5.4). In such situation $K^{\text{eff}}$ is a linear function of the matrix conductivity $K^{\text{eff}}(h) = K_E K_1(h)$ or $K^{\text{eff}}(h) = K_E K_2(h)$. The coefficient $K_E$ is constant and depends on the geometry. Thus, the local boundary value problem needs to be solved only once to obtain the whole $K^{\text{eff}}(h)$ curve.

For the considered isotropic geometries (squares, circles, cubes, spheres) the values of $K^{\text{eff}}$ obtained for weakly conductive inclusions correspond to the upper bound of Hashin–Shtrikman, while for the highly conductive inclusions $K^{\text{eff}}$ coincide with the lower bound of Hashin–Shtrikman. For the same volume fraction of inclusions the differences between spheres and cubes or between circles and squares seem rather insignificant. There exists, however, a difference between two-dimensional and three-dimensional geometries, which has been indicated by Hashin & Shtrikman (1962). Similarly, the results obtained for different spatial arrangements of spherical or cubic inclusions are very close, within the range of numerical error. Therefore, it can be concluded that for simple forms of inclusions the effective conductivity of the double-porosity media can be calculated as a function of the volume fraction of inclusions only.

The problem becomes more complicated for anisotropic geometry. Although our numerical analysis was limited to a simple two-dimensional case, it showed the importance of the anisotropy for the macroscopic transfer properties of the medium. Since many natural porous media exhibit anisotropy this effect should be taken into account in the macroscopic modeling. The homogenization method appears to be a convenient tool in this case. All the geometrical features of the period are taken into account in the model through the local boundary value problem. Therefore, the macroscopic properties obtained from homogenization enable us to reproduce accurately the macroscopic behavior of the medium.
Chapter 6

Examples of numerical solution of macroscopic problems

6.1 Introduction

In this chapter we present results of numerical simulations of the macroscopic boundary value problems for highly heterogeneous soils. The simulations were performed with three main objectives:

- to test the performance of the code DPOR-1D, described in Chapter 4;
- to validate the macroscopic models developed in Chapter 3 by comparison with the fine scale numerical solution;
- to compare the obtained results with other available models.

One way to evaluate the accuracy of the macroscopic model is the comparison with the fine scale numerical solution. In the fine scale solution the heterogeneous structure of the medium is explicitly represented and the local-scale equations are solved over the whole domain. Since such approach does not involve any up-scaling process it can be treated as the reference for the models obtained by homogenization. This type of simulations requires fine discretization (both in space and in time) in order to minimize the numerical errors and consequently the use of high-performance computers is necessary. Other possible method of verification of the model is comparison with experimental results, which is presented in Chapter 7.

The numerical tests were performed for three types of local geometry:

- Example A: medium with both highly conductive and weakly conductive sub-domain interconnected;
Example B: medium with weakly conductive inclusions embedded in highly conductive connected matrix;

Example C: medium with highly conductive inclusions embedded in weakly conductive matrix.

Examples A and B concern the local non-equilibrium flow model (Chapter 3, Section 2), which has been derived for the assumption that the highly conductive sub-domain is interconnected. They are taken from Lewandowska et al. (2004b). Example C refers to the model for soil with highly conductive inclusions (Chapter 3, Section 3). It has been presented in the paper by Lewandowska et al. (2004a).

All simulations concern infiltration in initially dry soil. Such problem often appears in practical applications. On the other hand it can be considered as a valuable test of the performance of the numerical solution, due to the presence of large gradients and the development of sharp wetting fronts.

6.2 Soil with the highly conductive sub-domain interconnected

6.2.1 Geometry and local hydraulic properties

Two different types of local geometry were considered. In Example A the more conductive regions have the form of vertical columns of square cross section, embedded in a weakly conductive interconnected matrix — Fig. 6.1. The medium is periodic in $X_1$ and $X_2$ directions. The periodicity in $X_3$ direction (which corresponds to the direction of macroscopic flow) is arbitrary. In Example B the less conductive medium forms horizontal parallelepipeds of square cross-section (Fig. 6.2). In this case we have 100 periods in the $X_3$ direction. The periodicity in $X_2$ direction is arbitrary. In each case the macroscopic problem can be represented as one-dimensional. It was solved for a 50 cm thick soil layer. The local flow problems are two-dimensional in both examples. The volume fractions of the sub-domains are nearly equal in both cases ($w_1 = 0.49$ and $w_2 = 0.51$ in Example A, $w_1 = 0.51$ and $w_2 = 0.49$ in Example B). Both materials are locally homogeneous and isotropic. We assume that the water retention curve $\theta(h)$ (Fig. 6.3) and the relative conductivity curve $K_r(h)$ (Fig. 6.4) are identical in both porous sub-domains. We are aware that such case is hardly encountered in nature, however we were interested the general performance of the model. Thus we imposed the conditions in such way that all assumptions underlying the model are satisfied. Consequently, we have the same relation for the capillary capacity $C(h)$ in the two
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Figure 6.1: Example A: Geometry of the medium and boundary conditions.

Figure 6.2: Example B: Geometry of the medium and boundary conditions.
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sub-domains. The values of the saturated conductivity differ by four orders of magnitude, $K_{s2} / K_{s1} = 10^{-4}$.

We used the van Genuchten – Mualem (Mualem, 1976; van Genuchten, 1980) hydraulic functions:

$$\theta = \theta_r + (\theta_s - \theta_r) \left[1 + (\alpha |h|^n)^{-m}\right]^{-m}$$

(6.1)

$$K = K_s \left\{ \frac{1 - (\alpha |h|^{-n}) \left[1 + (\alpha |h|^n)^{-m}\right]^2}{\left[1 + (\alpha |h|^n)^m\right]^{m/2}} \right\}^2$$

(6.2)

with the following parameters: $\theta_r = 0.045$, $\theta_s = 0.430$, $\alpha = 0.145 \text{ cm}^{-1}$, $n = 2.68$, $m = 1 - 1/n = 0.627$. Those parameters correspond to a typical sand as given by Carsel & Parrish (1988). The values of the saturated conductivities are $K_{s1} = 30 \text{ cm h}^{-1}$ and $K_{s2} = 0.003 \text{ cm h}^{-1}$ for sub-domains $\Omega_1$ and $\Omega_2$, respectively.

6.2.2 Macroscopic flow model and effective parameters

The macroscopic model obtained by homogenization (3.63) has the following one-dimensional form:

$$C^{eff} \frac{\partial h}{\partial t} - \frac{\partial}{\partial X_3} \left[ K^{eff} \frac{\partial}{\partial X_3} (h + X_3) \right] + \frac{1}{|\Omega|} \int_{\Omega_2} C_2 \frac{\partial h_2}{\partial t} = 0$$

(6.3)

where the integral source term is obtained from the solution of local-scale flow problem (3.55)–(3.56). The effective capillary capacity 3.64) is defined as:

$$C^{eff}(h) = w_1 C_1(h)$$

(6.4)

Since the flow is macroscopically one-dimensional, we need only one component of the effective conductivity tensor — $K_{33}^{eff}$, given by following formula:

$$K_{33}^{eff} = \frac{K_1^{(0)}}{|\Omega_1|} \int_{\Omega_1} \left(1 + \frac{\partial \chi_3}{\partial y_3}\right) d\Omega$$

(6.5)

where the function $\chi_3$ is obtained from the local boundary value problem (3.53)–(3.54).

The calculation of the effective parameters and the solution of the macroscopic problem were performed by DPOR-1D code, following the algorithm presented in Chapter 4. This solution will be referred to as DPH.

Example A

In Example A the effective capillary capacity is given by the following relation:

$$C^{eff}(h) = w_1 C_1(h) = 0.49 \ C_1(h)$$

(6.6)
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Figure 6.3: Examples A and B: Water retention function of sub-domain 1 $\theta_1(h)$ and effective water retention functions $\theta^{\text{av}}(h)$.

Figure 6.4: Examples A and B: (a) Effective capillary capacity $C^{\text{eff}}(h)$ and (b) effective conductivity $K^{\text{eff}}(h)$. 
The effective capillary capacity is shown in Fig. 6.4. In this example, due to the particular geometry the local boundary problem for the $\chi_3$ becomes:

$$
\frac{\partial}{\partial y_1} \left[ K_1^{(0)} \frac{\partial \chi_3}{\partial y_1} \right] + \frac{\partial}{\partial y_2} \left[ K_1^{(0)} \frac{\partial \chi_3}{\partial y_2} \right] = 0 \quad \text{in } \Omega_1 \quad (6.7)
$$

with the boundary condition

$$
\left[ K_1^{(0)} \frac{\partial \chi_3}{\partial y_1} \right] N_1 + \left[ K_1^{(0)} \frac{\partial \chi_3}{\partial y_2} \right] N_2 = 0 \quad \text{on } \Gamma \quad (6.8)
$$

Moreover $\chi_3$ has zero-valued volume average over $\Omega_1$ and it is periodic in $y_3$ direction. For this particular conditions the solution of (6.7)–(6.8) is straightforward and yields:

$$
\chi_3 = 0 \quad \text{and} \quad \frac{\partial \chi_3}{\partial y_3} = 0 \quad (6.10)
$$

Thus, from (6.5) one obtains the following expression for the effective conductivity:

$$
K_{\text{eff}}(h) = w_1 K_1(h) = 0.49 \, K_1(h) \quad (6.11)
$$

Note that in this particular case the effective conductivity is equal to the conductivity of the more conductive sub-domain multiplied by its volume fraction. The effective conductivity function is shown in Fig. 6.4.

**Example B**

The effective capillary capacity is given by the following formula

$$
C_{\text{eff}}(h) = w_1 C_1(h) = 0.51 \, C_1(h) \quad (6.12)
$$

The effective capillary capacity is shown in Fig. 6.4.

In this example the local boundary value problem, which defines the $\chi_3$ function is two-dimensional.

$$
\frac{\partial}{\partial y_1} \left[ K_1^{(0)} \left( \frac{\partial \chi_3}{\partial y_1} \right) \right] + \frac{\partial}{\partial y_3} \left[ K_1^{(0)} \left( 1 + \frac{\partial \chi_3}{\partial y_3} \right) \right] = 0 \quad \text{in } \Omega_1 \quad (6.13)
$$

with the condition:

$$
\left[ K_1^{(0)} \left( \frac{\partial \chi_3}{\partial y_1} \right) \right] N_1 + \left[ K_1^{(0)} \left( 1 + \frac{\partial \chi_3}{\partial y_3} \right) \right] N_3 = 0 \quad \text{on } \Gamma \quad (6.14)
$$
with the periodicity and normalization conditions:

\[ \chi_3(y_3 = 0) = \chi_3(y_3 = l_1) \quad (6.15) \]
\[ \chi_3(y_3 = 0) = \chi_3(y_3 = l_3) \quad (6.16) \]
\[ \int_{\Omega_1} \chi_3 \, d\Omega = 0 \quad (6.17) \]

where \( l_1 \) and \( l_3 \) denote size of the period in \( y_1 \) and \( y_3 \), respectively. The numerical solution of (6.13)–(6.17) (DPOR_1D code) and application of the formula (6.5) yields:

\[ K^{\text{eff}}(h) = w_1 K_1(h) = 0.328 K_1(h) \quad (6.18) \]

The coefficient appearing in the expression (6.18) is smaller than the volume fraction of the highly conductive sub-domain. The effective conductivity function is shown in Fig. 6.4.

### 6.2.3 Other existing models

#### The fine scale solution (FS)

We assume that the behavior of an heterogeneous medium can be adequately reproduced (in the range of numerical approximations) by solving the local-scale Richards equation:

\[ C \frac{\partial h}{\partial t} - \nabla \cdot (K \nabla (h + Y_3)) = 0 \quad (6.19) \]

Equation (6.19) is written with respect to the local spatial variable \( Y \). The solution is performed on a fine numerical grid with explicit representation of the local heterogeneity. The hydraulic conductivity of the medium is discontinuous at the interfaces between the highly and weakly conductive sub-domains.

The fine scale solution was obtained using the SWMS_3D code (Šimůnek et al., 1995). The code can be used to simulate three-dimensional flow and transport in unsaturated soils. The numerical algorithm applied in SWMS_3D is based on the finite element method with fully implicit discretization in time.

#### The model of Gerke and van Genuchten (1993a) (DPGG)

The dual-porosity model of Gerke & van Genuchten (1993a) is described in more detail in Chapter 2. The model consists of two macroscopic equations (2.25)–(2.26):

\[ C_1 \frac{\partial h_1}{\partial t} - \nabla \cdot (K_1 \nabla (h_1 + X_3)) + \frac{Q}{w_1} = 0 \quad (6.20) \]
\[ C_2 \frac{\partial h_2}{\partial t} - \nabla \cdot (K_2 \nabla (h_2 + X_3)) - \frac{Q}{w_2} = 0 \quad (6.21) \]
coupled by a first-order exchange term:

\[ Q = \frac{\beta}{a^2} \gamma_w K_a(h) (h_1 - h_2) \]  

(6.22)

where \( \beta \) is a geometry dependent coefficient, \( a \) is the distance from center to surface of low conductive block of medium \( 2 \), \( \gamma \) is an empirical coefficient and \( K_a \) is the conductivity of the interface between sub-domain \( 1 \) and \( 2 \). The interface conductivity \( K_a \) was evaluated from the following formula:

\[ K_a = \frac{1}{2} (K_a(h_1) + K_a(h_2)) \]  

(6.23)

It was assumed that the function \( K_a(h) \) is equal to the conductivity of the weakly conductive medium \( K_2(h) \). In Example A the following values of parameters were used: \( \gamma = 0.4 \), \( a = 0.75 \) cm and \( \beta = 2.82 \), whereas in Example B \( \gamma = 0.4 \), \( a = 0.175 \) cm and \( \beta = 11 \). The value of \( \gamma \) was chosen following the suggestions presented in (Gerke & van Genuchten, 1996).

In order to obtain the solution of (6.20)–(6.21), we developed a numerical code (DPGG_1D). A fully implicit finite difference scheme, similar to the one described in Chapter 4, was used for the discretization of the system (6.20)–(6.21). The nonlinear equations were solved by the Picard method. In this case the resulting system of linear algebraic equations has banded matrix of coefficients with bandwidth equal to 5, which can be effectively solved by a direct method similar to the Thomas algorithm (Section 4.4).

The single-porosity model (SP)

In the single-porosity model the weakly conductive sub-domain is assumed to be inactive. The macroscopic equation is following:

\[ C^{eff} \frac{\partial h}{\partial t} - \frac{\partial}{\partial X_3} \left[ K^{eff} \frac{\partial}{\partial X_3} (h + X_3) \right] = 0 \]  

(6.24)

where the effective parameters depend only on the parameters of the highly conductive matrix and the local geometry. They are defined according to (6.4) and (6.5). Note that the exchange of water between the two sub-domains is completely neglected. This model represents a limit case of the local non-equilibrium model (6.3) where the exchange term is equal to zero. We provided this solution in order to capture the influence of the weakly conductive sub-domain (double-porosity effect).

6.2.4 Initial and boundary conditions

Example A

In Example A the initial and boundary conditions represent the infiltration of water into a dry soil under a prescribed constant flux (Fig. 6.1). The value of the flux was chosen to be
less than $K_{s1}$ in order to keep unsaturated conditions during the flow:

$$h = -1000 \text{ cm} \quad -50 \text{ cm} \leq X_3 \leq 0, \quad t = 0$$

$$q = 12 \text{ cm} \, \text{h}^{-1} \quad X_3 = 0, \quad t \geq 0$$

The imposed flux represents mean value averaged over the cross section of the soil surface. It was assumed that the whole amount of water infiltrates into the more conductive sub-domain 1 (sub-domain 2 is effectively sealed at the surface). Thus, for the DPGG solution we imposed local infiltration rates $q_1 = 12 \text{ cm} \, \text{h}^{-1}/0.49 = 24.49 \text{ cm} \, \text{h}^{-1}$ in sub-domain $\Omega_1$ and $q_2 = 0$ in sub-domain $\Omega_2$. Similarly, in the FS solution with SWMS_3D code we imposed the infiltration rate equal to $24.49 \text{ cm} \, \text{h}^{-1}$ only on the part of surface occupied by sub-domain $\Omega_1$ and the flux was set to zero on the other part.

At the bottom boundary, the free drainage condition was imposed:

$$\frac{\partial h}{\partial X_3} = 0 \quad X_3 = -50 \text{ cm}, \quad t \geq 0$$

Example B

In Example B the initial and boundary conditions correspond to the infiltration into dry soil under constant pressure applied at the surface (Fig. 6.2):

$$h = -100 \text{ cm} \quad -50 \text{ cm} \leq X_3 \leq 0, \quad t = 0$$

$$h = -2 \text{ cm} \quad X_3 = 0, \quad t \geq 0$$

Similarly to the previous example, free drainage condition was imposed at the bottom of the column:

$$\frac{\partial h}{\partial X_3} = 0 \quad X_3 = -50 \text{ cm}, \quad t \geq 0$$

6.2.5 Numerical parameters

In Example A all numerical solutions were performed using uniform spatial discretization in $X_3$ direction ($\Delta X = 0.25 \text{ cm}$). The discretization of two-dimensional local flow problems in $Y_1$ and $Y_2$ direction for the DPH solution was uniform ($\Delta Y = 0.125 \text{ cm}$), whereas for the FS solution the spatial interval varied from $\Delta Y = 0.0625 \text{ cm}$ to $\Delta Y = 0.125 \text{ cm}$. In Example B the SP, DPGG and DPH solutions were obtained with $\Delta X = 0.5 \text{ cm}$. In the DPH solution each node corresponds to one inclusion. Each inclusion was discretized with $\Delta Y = 0.0175 \text{ cm}$. Due to the symmetry, the local problem is solved in a quarter of inclusion only. In case of fine scale solution we used variable spatial discretization with spatial step ranging from $\Delta Y = 0.0025 \text{ cm}$ to $\Delta Y = 0.06 \text{ cm}$ in each direction. All calculations were performed with
variable time step, with the initial value being as small as $10^{-12}$ h. The imposed accuracy was $\Delta h = 0.1$ cm. The real time of the numerical simulation varied considerably for different models. For the SP and DPGG solutions it was of the order of a few seconds, for the DPH approach — several hours and for the FS solution — up to 100 hours. All calculations were performed on comparable machines.

### 6.2.6 Results and discussion

#### Example A

The evolution of the mean water pressure head in sub-domain $\Omega_1$ at the bottom of the column ($X = 50$ cm) is shown in Fig. 6.5a. The mean water pressure head corresponds to the macroscopic capillary pressure for DPH and SP solutions, while for DPGG solution
Chapter 6. Examples of numerical solution of macroscopic problems

Figure 6.6: Evolution of the macroscopic flux $q$ at the bottom of the profile $X_3 = -50$ cm in Example A (a) and Example B (b) according to the model obtained by homogenization (DPH), the reference solution (FS), the Gerke and van Genuchten (DPGG) and simple porosity (SP) approaches.

It corresponds to the pressure head $h_1$ in the more conductive region. In FS solution it is calculated as an average over the part of cross section surface occupied by sub-domain $\Omega_1$. It can be seen that the DPH gives a solution very close to the fine scale solution (FS3D). The evolution of the capillary pressure head in the DPGG model is slightly different. The time evolution of the flux at the bottom of the layer is presented in Fig. 6.6a. The presence of the weakly conductive sub-domain slows down the propagation of the wetting front, which is clearly visible. The homogenized solution (DPH) coincides with the three-dimensional reference solution (FS). The DPGG approach gives a different solution. In that case the arrival of the wetting front is faster, but later on the flux takes longer time to reach a steady state. This difference can be clearly explained by comparing the values of the source term
in the DPGG and DPH models. The time evolution of these terms at different depths in the column is shown in Fig. 6.7a. We also provided the water exchange rates obtained from FS solution, calculated as the rate of variation of water content in sub-domain $\Omega_2$ with time. It can be seen that the water transfer rate in the DPGG model is significantly underestimated during the initial phase of infiltration, while during later stages of the process it is slightly overestimated. This problem was also shown by Gerke & van Genuchten (1993b). The flux in the double porosity soil reaches its steady state value considerably later compared to the single porosity example. This retardation, known as the tail effect, can be estimated by the normalized tail flux $q_T$ defined as:

$$q_T = \frac{q_S - q_D}{q_S}$$  \hspace{1cm} (6.25)
where $q_S$ and $q_D$ are the fluxes calculated from the simple porosity model and the double porosity models (DPH, DPGG or FS, respectively). Thus, the value of $q_T$ varies between 0 and 1, which indicates minimum and maximum value of the tail effect. Fig. 6.8a presents the evolution of $q_T$ at the bottom of the column with respect to the retardation time $t_R$, where $t_R = 0$ represents the time of appearance of the non-zero flux in the single porosity model (SP).

**Example B**

The evolution of the mean water pressure head in sub-domain $\Omega_1$ is presented in Fig. 6.5b and the evolution of the mean flux at the bottom of the column is presented in Fig. 6.6b. The slower propagation of the wetting front in the double porosity medium can be easily observed, as it was in Example A. The solution obtained from the DPGG approach is significantly different from the others. This can be partially explained by the fact that the estimation of the effective macroscopic conductivity of the more conductive sub-domain $\Omega_1$ in the DPGG model is proportional to its volume fraction only. As a result the steady state flux corresponding to the given boundary conditions is about 50% greater than the one obtained with the other solutions. The small discrepancy between the steady state flux obtained by DPH and FS calculations can be explained by numerical factors (different methods of spatial discretization and grid sizes). The time evolution of the exchange term along the column is shown in Fig. 6.7b. Again, the values from DPH, DPGG and FS models are compared. Note that the DPH solution is close to the reference solution, while the DPGG gives results that are very different qualitatively and quantitatively. The normalized tail flux $q_T$ as a function of the time $t_R$ is presented in Fig. 6.8b. In that case negative values obtained from the DPGG solution are due to the fact that the macroscopic flux in this model is considerably larger than the flux obtained from the single porosity (SP) approach.
Figure 6.8: Evolution of the normalized tail flux $q_T$ at $X_3 = -50$ cm according to the model obtained by homogenization (DPH), the reference solution (FS3D) and the Gerke and van Genuchten model (DPGG); $q_T$ is the relative difference between the flux in simple (SP) and double porosity models; the retardation time $t_R = 0$ corresponds to the arrival of the wetting front in the simple porosity model. (a) Example A, (b) Example B.
6.3 Soil with highly conductive inclusions

6.3.1 Geometry and local hydraulic properties

The problem concerns one-dimensional vertical infiltration into a heterogeneous soil layer of the thickness $L = 50$ cm. The domain is composed of highly conductive porous parallelepipeds of square section (sub-domain $\Omega_1$) arranged horizontally in a porous low conductive matrix (sub-domain $\Omega_2$). The vertical cross-section of the soil is presented in Fig. 6.9. The medium shows a periodic structure in the directions $X_1$ and $X_3$. The periodicity in the $X_2$ direction is arbitrary. There are 100 periods in the vertical direction $X_3$ that yields $\varepsilon = 0.01$. The volumetric fractions of the two sub-domains are $w_1 = 0.49$ and $w_2 = 0.51$, respectively. Both materials are locally homogeneous and isotropic.

Similarly to the previous examples it was assumed that the hydraulic characteristics in both sub-domains are described by the van Genuchten - Mualem functions. We used the same parameters as in Examples A and B, namely $\theta_r = 0.045$, $\theta_s = 0.43, \alpha = 0.145 \text{ cm}^{-1}$, $n = 2.68$, $K_{s1} = 30 \text{ cm h}^{-1}$. In the sub-domain $\Omega_2$, the saturated hydraulic conductivity is scaled by the factor 100, $K_{s2} = 0.3 \text{ cm h}^{-1}$, while other parameters are unchanged. Therefore, conditions concerning the contrast between the parameters are satisfied.
6.3.2 Macroscopic model and effective parameters

The one-dimensional form of the macroscopic flow equation (3.110) with the effective parameters $C^{\text{eff}}$ and $K^{\text{eff}}$ is written as follows (3.110):

$$C^{\text{eff}} \frac{\partial h}{\partial t} - \frac{\partial}{\partial X_3} \left[ K^{\text{eff}} \frac{\partial}{\partial X_3} (h + X_3) \right] + \frac{1}{|\Omega|} \int_{\Omega_2} C_2 \frac{\partial h_2}{\partial t} = 0 \quad (6.26)$$

In this example both sub-domains are characterized by the same retention function. Therefore, the effective water capacity is equal to the local water capacity

$$C^{\text{eff}}(h) = w_1 C_1(h) + w_2 C_2(h) \quad (6.27)$$

The function is presented in Fig. 6.10.

Similarly to the previous examples, the only required component of the effective conductivity tensor is $K^{\text{eff}} = K^{\text{eff}}_{33}$ corresponding to the vertical direction, which is defined as:

$$K^{\text{eff}}_{33} = \frac{1}{|\Lambda_3|} \int K^{(0)}_2 \left( I_{33} - \frac{\partial \chi_3}{\partial y_3} \right) d\Lambda \quad (6.28)$$

where $\Lambda_3$ is the cross section of the period normal to the $y_3$ direction. Due to the arbitrary periodicity in the $X_2$ direction, the function $\chi_3$ is independent of $y_2$ and the local boundary value problem is two-dimensional. In order to find the function the local boundary value problem should be solved in the sub-domain $\Omega_2$. It takes the form of a Poisson-type equation:

$$\frac{\partial}{\partial y_1} \left[ K^{(0)}_2 \left( - \frac{\partial \chi_3}{\partial y_1} \right) \right] + \frac{\partial}{\partial y_3} \left[ K^{(0)}_2 \left( 1 - \frac{\partial \chi_3}{\partial y_3} \right) \right] = 0 \quad \text{in } \Omega_2 \quad (6.29)$$

with the boundary condition:

$$\chi_3 = y_3 \quad \text{on } \Gamma \quad (6.30)$$

and periodic boundary conditions at the outer boundaries. The local boundary value problem was solved using DPOR_1D code. Application of the definition (6.28) leads to the following formula for the effective conductivity:

$$K^{\text{eff}}(h) = 3.055 \, K_1(h) \quad (6.31)$$

As it can be seen the effective hydraulic conductivity is over three times greater than the conductivity in the porous matrix $K_2$. The function is presented in Fig. 6.10.

The solution of the macroscopic equation (6.26) was performed using DPOR_1D code. It will be referred to as DPH solution.
6.3.3 Other existing models

The fine scale solution

Similarly to the Examples A and B we performed a direct two-dimensional simulation of the unsaturated flow in heterogenous medium (FS solution). In this case we used the SWMS_2D code (ˇSimůnek et al., 1994), based on similar numerical formulation as SWMS_3D.

The single-porosity model

For the purposes of comparison, a single-porosity (SP) solution was also provided. In this approach we neglect the presence of highly conductive inclusions. The soil is treated as homogeneous and the hydraulic parameters are equal to the parameters of the weakly conductive matrix.

6.3.4 Initial and boundary conditions

The initial and boundary conditions are similar to those from Example B. They describe the infiltration into initially dry soil under constant water pressure head (Fig. 6.9):

\[
\begin{align*}
    h &= -100 \text{ cm} & -50 \text{ cm} \leq X_3 &\leq 0, & t &= 0 \\
    h &= -2 \text{ cm} & X_3 &= 0, & t &\geq 0
\end{align*}
\]
Similarly to the previous examples, free drainage was imposed at the bottom of the column:

\[ \frac{\partial h}{\partial X_3} = 0 \quad X_3 = -50 \text{ cm}, \quad t \geq 0 \]

### 6.3.5 Numerical parameters

The DPH calculations were performed on a uniform grid with \( \Delta X = 0.5 \text{ cm} \). The time step varied from \( 10^{-9} \text{ h} \) to 1 h. The accuracy of the solution was specified in terms of the absolute capillary pressure head error, \( \Delta h = 0.1 \text{ cm} \). The total time of the run was about 30 s on PC with 2GHz processor. In the fine scale solution, the two-dimensional domain was discretized with a non-uniform structured grid (\( \Delta Y \) varied from to 0.005 cm to 0.06 cm). The time step was allowed to vary within the range \( 10^{-9} \text{ h} \) to 1 h. The accuracy was specified in terms of the absolute water content error, \( \Delta h = 0.1 \text{ cm} \). The total time of the run was about 240 h on a workstation with DS20 HP/Compaq processors (MIRAGE, Grenoble).

### 6.3.6 Results and discussion

In Fig. 6.11 the local water pressure head along the vertical symmetry axis of the column obtained from the DPH model and FS model are compared. It can be seen that the DPH and the FS solutions are close to each other. It can also be seen that the local variations of the capillary pressure head in the two regions (FS solution) with respect to the "homogenized solution" (DPH solution) are small. It confirms the local equilibrium conditions of the flow.
**Figure 6.12:** Example C: Evolution of the water pressure head in the middle ($X_3 = -25\ cm$) and at the bottom ($X_3 = -50\ cm$) of the column obtained from homogenization (DPH) and fine scale solution (FS). For the FS solution volume averages of $h$ over more conductive $\Omega_1$ and less conductive $\Omega_2$ sub-domain of the period are presented.

**Figure 6.13:** Example C: Evolution of the mean flux obtained from homogenization (DPH), fine scale solution (FS) and single porosity (SP) model in the middle ($X_3 = -25\ cm$) and at the bottom ($X_3 = -50\ cm$) of the column.
The small oscillations around the average value of the water pressure head are caused by the action of the gravity force at the interfaces between the weakly and highly conductive regions. They are of the order 0.25 cm. This result confirms our assumption ($O(\varepsilon)$). Nevertheless, gravity contributes to the acceleration of the water front in a considerable way and this effect seems to be correctly described by the presented model. The evolution of the water pressure head in the middle ($X_3 = -25$ cm) and at the bottom of the column ($X_3 = -50$ cm) are presented in Fig. 6.12. For the FS solution the volume averages of the water pressure head $h$ over the $\Omega_1$ and $\Omega_2$ sub-domains of the period were calculated. It can be clearly seen that the pressure in the two regions equilibrates very quickly. The macroscopic fluxes at $X_3 = -25$ cm and $X_3 = -50$ cm from the DPH and FS models are shown in Fig. 6.13. The two solutions are very close to each other, which confirms the validity of the theoretical model presented in Chapter 3. The comparison of the DPH model with the SP model gives the idea of the acceleration of the infiltration process caused by the presence of highly conductive inclusions. The flux is smaller and the velocity of the wetting front is also much less in SP solution than in the case of the medium with inclusions (DPH solution).

6.4 Summary

We presented numerical solutions of the two macroscopic models of flow developed by the method of homogenization. The simulations concerned three different soil geometries. The results were compared to the fine scale solution, treated as the reference. We should note however that the fine scale solutions were difficult to obtain, especially in Example B and C. This was due to large number of heterogeneities in the considered domain (100 periods) and due to the sharp-front infiltration process. Note that this type of simulation requires the use of powerful computers. In our tests we encountered several difficulties (lack of convergence, oscillations). Thus, the fine scale solution can be treated as an approximation of the exact solution of the local-scale equations since it is influenced by some numerical errors. Nevertheless, in all cases we obtained a good agreement between the fine scale solution and the solution from homogenization. It confirms, that the homogenization method provides efficient tools for modeling unsaturated flow in highly heterogeneous soils. The time required for the simulation by DPOR-1D code was usually 10 to 20 times less than for the corresponding fine scale solution by SWMS_2D or SWMS_3D code.

In the first two examples the non-equilibrium model obtained by homogenization was compared with the phenomenological dual-porosity model proposed by Gerke & van Genuchten (1993a). For a simple local geometry (Example A), the Gerke and van Genuchten phenomenological model gives results close to the double porosity model obtained from the
homogenization approach (in terms of the mean water pressures and fluxes). This is valid, despite of the approximative expression for the exchange term. In the case of a more complex local geometry (Example B), the comparison between the Gerke and van Genuchten model and the double porosity homogenization model showed very different results. The observed differences can be explained by an inadequate in this case estimation of the effective hydraulic conductivity and of the source term proposed in the Gerke and van Genuchten model. One should note that more other expressions for the exchange term have been proposed in literature (Zimmerman et al., 1996, e.g.). Nevertheless, the DPGE model seems to be the most widespread (Šimůnek et al., 2001; Gerke & Köhne, 2004) and for this reason we decided to use it in the comparative calculations. Note also that the two-equation model of the type proposed by Gerke & van Genuchten (1993a) cannot be applied to describe the flow in soils with highly conductive inclusions (Example C).
Chapter 7

Comparison of the theoretical model with experimental results

7.1 Introduction

One of the major problems concerning the modeling of unsaturated flow in double-porosity soils is the validation of the macroscopic models. The validation should be preferably carried out by means of an experiment. The experimental data available in literature are often difficult to use. Actually, in order to validate the macroscopic model one should have full information on the local geometry of the medium and hydraulic characteristics of the two sub-domains, which is hardly available, especially in the case of field experiments. One possible solution is to perform experiments on a model double-porosity medium, where the components are arranged in a regular manner and their properties can be measured independently.

For the purposes of our analysis we used the results of infiltration experiments in double-porosity medium carried out in Laboratoire LTHE (Grenoble, France) (Gorczewska, 2003; Lewandowska et al., 2004c). The considered medium consisted of a mixture of fine sand and sintered clayey spheres arranged in a periodic manner. The hydraulic characteristics of each material were obtained from independent infiltration tests by inverse analysis. They were used to calculate the effective parameters of the double-porosity model by solving first the local boundary value problem. Then the macroscopic boundary value problem was solved. The experiments with the double-porosity medium dealt with infiltration under constant pressure head into initially dry medium. The same kind of tests was performed in each material separately, in order to keep similar initial and boundary conditions and to avoid the possible influence of hysteresis.

In the following sections we present the infiltration experiments performed in sand, sin-
Chapter 7. Comparison of the theoretical model with experimental results

tered clayey material and double-porosity medium, identification of the hydraulic parameters for each of the two materials by inverse analysis, calculation of the effective parameters of the double-porosity medium and comparison between the experimental results and the numerical simulations.

7.2 Experiments

7.2.1 Material

The double-porosity medium used in the experiments was a mixture of Hostun sand HN38 (Flavigny et al., 1990) and spheres made of sintered clayey material (Fig. 7.1). The chemical composition of the sand is mainly quartz. The skeleton density is \( \rho_s = 2.65 \text{ g cm}^{-3} \). The grain distribution is relatively uniform (Fig. 7.2), with 51.2% of particles between 100 \( \mu \text{m} \) and 200 \( \mu \text{m} \), the mean grain diameter being 162 \( \mu \text{m} \). A series of laboratory standard compaction tests performed in a cylinder (12.6 cm high and 7.1 cm in diameter) gave porosity values ranging from \( m_{1\text{min}} = 0.412 \) to \( m_{1\text{max}} = 0.538 \).

The sintered clayey spheres were made by hand in a pottery workshop. The origin of the clay was La Bisbal, Spain. It was washed and then fired at temperature of 1000°C, following an old traditional technology. The analysis by electronic scanning microscope showed that the clay material was relatively homogeneous, with no skin effect of reduced porosity close to the surface of the spheres. The mercury porosimetry test gave the porosity value of \( m_2 = 0.376 \), and the mean pore size around 0.7 \( \mu \text{m} \). The skeleton specific density obtained from mercury test is \( \rho_{s2} = 3.01 \text{ g cm}^{-3} \) and the dry bulk density \( \rho_{d2} = 1.88 \text{ g cm}^{-3} \). The spheres were of relatively uniform diameter with an average value of \( 2R = 6.4 \text{ mm} \). Small quantities of spheres of diameter as small as 4.3 mm and as large as 9.4 mm were observed. Assuming that the characteristic size of the sand pores was of the same order of magnitude as the size of the grains, the ratio of the pore sizes of clayey material and sand is of the order 1 : 230.

7.2.2 Experimental setup

Infiltration tests were performed in a clear acrylic column (60 cm high and 8 cm in inner diameter — Fig. 7.3), in which the porous material was placed layer by layer, each layer being mechanically compacted in a controlled and regular manner. A tension disc infiltrometer was placed on the surface of the column. The disc diameter was equal to that of the column, ensuring one-dimensional vertical flow. The infiltrometer consisted of an alimentation tube and a Mariotte bottle which allowed to apply a constant value of pressure head at the
Figure 7.1: Porous materials used in the experiments: a) macroscopic view of sand and sintered clayey spheres; b) sand grains (scanning microscope, zoom 50); c) cross-section of a clayey sphere (scanning microscope, zoom 200).
surface. The amount of water infiltrating into the column as a function of time was manually monitored. The accuracy of the measurements was estimated at $+/- 0.6$ mm of water. The base of the column was maintained at the atmospheric pressure (free drainage). The porous medium was supported by a metal grid covered with a semi-permeable membrane. The water was allowed to flow out through the membrane into a recipient placed on a balance connected via a data-logger (Campbell Scientific Ltd CR 10X) to a computer which registered the outflow water mass during the experiments in the double-porosity medium. For the experiments conducted in sand, the outflow measurements were taken manually. The maximum error of observations was 1 g, which corresponds to an accuracy of $+/- 0.2$ mm of water. The room temperature varied between 23–24$^\circ$C.

### 7.2.3 Experiments in sand

In order to obtain the hydraulic characteristics of sand two experiments (Tests 1 and 2) were carried out using the setup described above. In each test the column was filled up with air-dry sand one day before the experiment. The initial volumetric water content was smaller than 0.001 (measured by a standard oven-drying procedure). The sand was put into column in layers of about 1 cm and each layer was compacted in order to obtain the same
sand porosity as it was in the experiments carried out with the double-porosity medium. We obtained $m_1 = 0.399$ in Test 1 and $m_1 = 0.407$ in Test 2. The pressure head imposed by the infiltrometer at the inlet of the column was $h_{surf} = -0.1$ cm of water. The cumulative infiltration and discharge volumes of water were registered manually. The breakthrough times, corresponding to the appearance of the first water drop at the outlet of the column was 3000 s in Test 1 and 2490 s in Test 2. In each case the infiltration was continued until the outflow reached a steady state regime (within the precision of the observations) and then beyond that time, until the supply tube was empty. At the end of each experiment the final water content $\theta_f$ was calculated from the difference between cumulative water inflow and outflow. The obtained values ($\theta_f = 0.338$ in Test 1 and $\theta_f = 0.346$ in Test 2) were significantly smaller than the porosity. It indicates that a fraction of pores was inaccessible for water or some quantity of air remained entrapped in the sand column as it has been commonly reported by various authors (e.g. Touma & Vauclin, 1986; Šimůnek et al., 2001, among others).
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7.2.4 Experiments in sintered clayey material

An infiltration experiment was carried out in a cylinder (25.9 cm high, 5.25 cm in diameter) made of the same sintered clayey material as the spheres (Test 3). A small infiltrometer with a 5 cm -diameter disc was placed on the top of the cylinder. The lateral surface of cylinder was isolated to avoid evaporation losses and by-pass flow. The material was air-dry and the initial volumetric water content was about 0.004. The applied water pressure head was \( h_{surf} = -0.1 \text{ cm} \). The volume of infiltrated water was registered manually. The experiment lasted about 60 h. After about 20 h visible wetting of the bottom surface of the cylinder was observed. However, no measurable amount of water flowing out was registered.

7.2.5 Experiments in double-porosity medium

Three replications of infiltration experiments were successively carried out in the double-porosity medium (Tests 4, 5 and 6), using the setup described in Section 7.2.2. Before each test, the column was filled up with sand and spheres in a controlled manner. Both materials were initially air-dry. The spheres were put layer by layer in such a way that they were touching each other. In each layer the void space between spheres was carefully filled with sand, which was then compacted. In that way a periodic arrangement was obtained. The volumetric fractions of spheres and sand, as well as the porosity of sand are given in Table 7.1. Small values of coefficient of variation indicate a satisfying reproducibility of the way the column was filled up with the double-porosity medium. Consequently, the following mean values were retained: volumetric fraction of sand \( w_1 = 0.445 \), volumetric fraction of spheres \( w_2 = 0.555 \) and porosity of sand \( m_1 = 0.405 \).

The pressure head \( h_{surf} = -0.1 \text{ cm} \) of water was imposed at the top of the column by means of the infiltrometer. The amount of water emanating from the disc was registered manually. The cumulative mass of water flowing out of the base of the column was continuously monitored. The breakthrough times were estimated at: 5460 s, 6000 s and 5970 s for Test 4, 5 and 6 respectively (Table 7.1). Each infiltration test lasted about 10 h and the steady state flow regime was reached, at least within the precision of measurements. The final water content varied between 0.29 and 0.3 (Table 7.1). During the experiments the position of the wetting front was visually recorded.
Table 7.1: Characteristics of the experiments performed in the double-porosity medium. CV is the coefficient of variation.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Test 4</th>
<th>Test 5</th>
<th>Test 6</th>
<th>Mean</th>
<th>CV [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volumetric fraction of sand, $w_1$ [-]</td>
<td>0.447</td>
<td>0.444</td>
<td>0.443</td>
<td>0.445</td>
<td>0.47</td>
</tr>
<tr>
<td>Volumetric fraction of spheres, $w_2$ [-]</td>
<td>0.553</td>
<td>0.556</td>
<td>0.557</td>
<td>0.555</td>
<td>0.37</td>
</tr>
<tr>
<td>Sand porosity, $m$ [-]</td>
<td>0.410</td>
<td>0.401</td>
<td>0.405</td>
<td>0.405</td>
<td>1.23</td>
</tr>
<tr>
<td>Final water content, $\theta_f$ [-]</td>
<td>0.290</td>
<td>0.290</td>
<td>0.300</td>
<td>0.293</td>
<td>1.97</td>
</tr>
<tr>
<td>Breakthrough time, [s]</td>
<td>5460</td>
<td>6000</td>
<td>5970</td>
<td>5810</td>
<td>5.20</td>
</tr>
</tbody>
</table>

7.3 Hydraulic characteristics of sand and sintered clayey material

7.3.1 Inverse analysis

It was assumed that both porous materials were adequately characterized by the van Genuchten – Mualem (Mualem, 1976; van Genuchten, 1980) closed-form relations:

\[
\theta = \theta_r + (\theta_s - \theta_r) \left[1 + (\alpha |h|)^n\right]^{-m}
\]

(7.1)

\[
K = K_s \frac{1 - (\alpha |h|)^n \left[1 + (\alpha |h|)^n\right]^{-m}}{\left[1 + (\alpha |h|)^n\right]^{m/2}}
\]

(7.2)

where $\theta_r$ and $\theta_s$ are the residual and saturated volumetric water content respectively, $K_s$ is the saturated hydraulic conductivity, $\alpha$, $n$ and $m$ are empirical constants ($m = 1 - 1/n$).

The total number of hydraulic parameters to be determined is equal to 5 for each material. The hydraulic functions can be obtained from direct measurements or by the inverse analysis. We used the latter approach, since it enables us to identify parameters corresponding to the wetting process from transient infiltration experiment. Most of the direct methods concerns steady-state flow and the drainage conditions.

The inverse analysis becomes routinely used for flow in unsaturated soils (Hopmans et al., 2002). This technique has been applied to one-step (Kool et al., 1985) and multi-step outflow experiments, infiltration from tension disc infiltrometers (Šimůnek & van Genuchten, 1996, 1997; Šimůnek et al., 1999) and upward flow (Hudson et al., 1996). One of the major problems arising in the inverse analysis is the non-uniqueness of the solution (Hornung, 1983). It means that very different set of parameters can give good approximation of the experimental results, especially when many parameters are fitted on a small data set (e.g. cumulative infiltration curve only). It is recommended (Šimůnek & van Genuchten, 1996;
Hopmans et al., 2002) to estimate parameters from independent measurements whenever possible and thus to reduce the number of fitted parameters.

In our study the HYDRUS-1D code (Šimůnek et al., 1998) was used to identify by an inverse procedure the hydraulic parameters of sand and clayey material from measured infiltration data. This was performed by minimizing the following objective function $\Phi$ expressed as:

$$\Phi(b) = \sum_{i=1}^{N} [I_{in}^{*} - I_{in}(b)]^2 + \sum_{j=1}^{M} [I_{out}^{*} - I_{out}(b)]^2$$  \hspace{1cm} (7.3)

where $b$ denotes the optimized parameter vector, $I_{in}^{*}$ and $I_{out}^{*}$ are measured cumulative infiltration and discharge amounts respectively, $I_{in}(b)$ and $I_{out}(b)$ are the corresponding simulated values for a given set of parameters. $N$ and $M$ are the numbers of infiltration and discharge measurements respectively. No weighting of the input data was considered and the Marquardt – Levenberg (Marquardt, 1963) algorithm was used for the minimization of function (7.3).

7.3.2 Sand

Conditions

For the Test 1 and 2, the measured cumulative infiltration and outflow values as function of time are presented in Figs 7.4 and 7.5 respectively. The number of optimized parameters was two, namely $\alpha$ and $n$, the remaining three ($\theta_r$, $\theta_s$ and $K_s$) having been estimated from additional considerations briefly exposed below.

We considered that $\theta_r = 0$. It can be justified by the fact that it should be less than the initial water content $\theta_{init}$, which was measured in air-dry conditions to be very small, $\theta_{init} < 0.001$. The volumetric water content at saturation $\theta_s$ was assumed to be equal to the final water content measured at the end of each test which is less than the porosity. The hydraulic conductivity at saturation $K_s$ was determined from an independent falling head test carried out in completely saturated conditions. The resulting value $K_s = 2.76 \times 10^{-3}$ cm/s was found to be close to the slopes of the cumulative inflow and outflow curves, measured when the steady state was attained. Consequently, in the inverse procedure, $K_s$ was set to be equal to the slope of the cumulative discharge curve measured in each Test (see Table 7.2). The HYDRUS-1D code was run with the following boundary conditions: $h_{surf} = -0.1$ cm of water at the inlet and free drainage ($\frac{\partial h}{\partial X} = 0$) at the outlet of the column. The initial condition was arbitrary prescribed at $h_{init} = -1000$ cm of water. After fitting we obtained initial value of volumetric water content smaller than 0.001, which corresponds to the experimental conditions.
Chapter 7. Comparison of the theoretical model with experimental results

Figure 7.4: Measured and calculated values of cumulative infiltration in sand and double-porosity medium.

Results

The inverse analysis was applied to Test 1 and Test 2 separately. The corresponding contour lines of the objective function $\Phi$ as function of the fitted parameters $\alpha$ and $n$ for are presented in Fig. 7.6. It can be seen that the surface of $\Phi$ shows a complex pattern with no well-defined global minimum. This makes the uniqueness of the solution questionable. Therefore, the inverse procedure was repeated for several different initial values of the searched parameters. In each run, either the same minima were obtained or the solution was found to be unstable. Consequently, the values of $\alpha$ and $n$ given in Table 7.2 for both tests were considered as the best estimates of the parameters of the van Genuchten – Mualem functions. They seem to be physically reasonable, by comparison with data reported in the literature for fine sand (Haverkamp et al., 1998). In the following, the arithmetic means of the parameters reported in Table 7.2 were retained. The resulting fitted cumulative infiltration and discharge as function of time are given in Figs 7.4 and 7.5. The corresponding retention, capacity and conductivity curves calculated from equations (7.1) and (7.2) are plotted in Fig. 7.7a, 7.7b and 7.8 respectively.
Chapter 7. Comparison of the theoretical model with experimental results

Figure 7.5: Measured and calculated values of the cumulative outflow in sand and double-porosity medium.

Table 7.2: Parameters of the van Genuchten – Mualem model for sand and sintered clayey material. Optimized values are printed in bold.
Chapter 7. Comparison of the theoretical model with experimental results

Figure 7.6: Contour lines of the objective function $\Phi \ [cm^2]$ for sand. The minimum is indicated by a marker.

Figure 7.7: (a) Retention function and (b) capillary capacity function of sand, sintered clayey material and the double-porosity medium.
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7.3.3 Sintered clayey material

Conditions

In the inverse procedure the cumulative infiltration curve measured in Test 3 (Fig. 7.9) was used. Three hydraulic parameters were optimized: $\alpha$, $n$ and $K_s$. The residual water content was set at $\theta_r = 0$. The $\theta_s$ value was obtained from an additional series of 8 saturation experiments. In those experiments, the porous spheres were put into free water and left until their saturation was reached. The final volumetric water content varied from 0.283 to 0.30, with a mean value of $\theta_f = 0.295$. Note that this value is significantly less than the porosity obtained by mercury porosimetry test ($m = 0.376$). We assumed that $\theta_f$ corresponds to the fraction of pores effectively accessible to water during infiltration and consequently $\theta_s$ was set at $\theta_s = \theta_f = 0.295$.

According to the experimental conditions the boundary values used in the inverse modeling were: $h_0 = -0.1$ cm at the surface of the cylinder and free drainage ($\frac{\partial h}{\partial X_3} = 0$) at the bottom. The imposed initial condition was the same as for the sand ($h_{\text{init}} = -1000$ cm of water) since the hydraulic parameters of both materials were used in the double-porosity medium.
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model which assumes initial equilibrium of pressure between the two sub-domains.

Results

The objective function $\Phi$ shows a well defined unique minimum (Fig. 7.10). The corresponding hydraulic parameters are given in Table 7.2 and the resulting fitted cumulative infiltration is plotted in Fig. 7.9. The values appear different from those reported in the literature for clay soils (Haverkamp et al., 1998). As a matter of fact it can be expected that the thermal treatment of clay caused some physical and chemical transformations of the material which have certainly influenced its hydraulic behavior. For example, the saturated hydraulic conductivity is of the same order of magnitude as values reported in the literature for bricks (Hall & Hoff, 2003). Also, it is worthwhile to note that the optimized conductivity approximately corresponds to the value of the slope of the cumulative discharge measured when the steady state regime was reached, $K_s = 1.11 \times 10^{-5}$ cm/s. The resulting retention and conductivity curves for clayey material are reported in Figs 7.7 and 7.8 respectively. Note that the initial water content $\theta_{\text{init}}$ corresponding to $h_{\text{init}} = -1000$ cm is about 0.02, which is slightly higher than the measured value ($\theta_{\text{init}} = 0.004$).
Chapter 7. Comparison of the theoretical model with experimental results

Figure 7.10: Contour lines of the objective function $\Phi \ [\text{mm}^2]$ for sintered clayey material. The minimum is indicated by a marker.

7.4 Numerical simulations

7.4.1 Macroscopic model

The numerical simulation of the infiltration experiments was performed according to the mathematical model of the local non-equilibrium flow in unsaturated double-porosity medium presented in Chapter 3 (Section 3.3) which reads for 1D vertical flow:

$$C^{eff} \frac{\partial h}{\partial t} - \frac{\partial}{\partial X_3} \left[ K^{eff} \frac{\partial}{\partial X_3} (h + X_3) \right] + \frac{1}{|\Omega|} \int_{\Omega} C_2 \frac{\partial h_2}{\partial t} = 0 \quad (7.4)$$

The value of the integral source term $\int_{\Omega_2} C_2 \frac{\partial h_2}{\partial t}$ is obtained from the solution of local-scale flow equations, which in our case are written in spherical coordinates:

$$\frac{\partial \theta_2}{\partial t} - \frac{\partial}{\partial r} \left( K_2 \frac{\partial h_2}{\partial r} \right) - \frac{2}{r} \left( K_2 \frac{\partial h_2}{\partial r} \right) = 0 \quad (7.5)$$

The calculations were carried out using the DPOR-1D code (see Chapter 4). They were performed in two steps: (i) determination of the effective parameters and (ii) solution of the macroscopic boundary value problem.

7.4.2 Determination of the effective parameters

The double-porosity medium is represented as a periodic arrangement of spheres embedded in sand and touching each other (within each layer). The successive layers of spheres are "staggered", which allows compacting. For this type of geometry, the volumetric fraction of spheres ($w_2$) can vary between 0.524 and 0.740 according to the distance between neighboring
layers. The geometry of the period was assumed to correspond to the one for which the volumetric fraction is equal to $w_2 = 0.555$. This is an average value of the volume fraction of spheres measured in the three experiments (Table 7.1). The geometry used for the solution of the local problem is shown in Fig. 7.11. The dimensions of the period are $6.4 \, \text{mm} \times 6.4 \, \text{mm} \times 12.08 \, \text{mm}$.

Both materials were assumed to be locally homogeneous and isotropic. In order to calculate the effective conductivity tensor the local boundary value problem was solved. Since the problem is macroscopically one-dimensional, $K_{33}^{e\!f\!f}$ is the only component required to solve the macroscopic flow equation. The solution was obtained with DPOR–1D code. A dense grid of $101 \times 101 \times 191$ nodes was used in order to correctly approximate the spherical shapes. Fig. 7.12 presents the function $\chi_3$ and its gradient $\left[ \frac{\partial \chi_3}{\partial Y_3} + 1 \right]$ obtained from the solution of the local boundary value problem. We show the vertical cross-section of the period along the diagonal of its base ($Y_1 = Y_2, Y_3$). Using the obtained values of $\chi_3$ the effective hydraulic conductivity was calculated from equation as:

$$K^{e\!f\!f}(h) = 0.308 \, K^{e\!f\!f}(h)$$  \hspace{1cm} (7.6)

The effective water capacity was calculated as:

$$C^{e\!f\!f}(h) = w_1 \, C_1(h) = 0.445 \, C_1(h)$$  \hspace{1cm} (7.7)
In equations (7.6) and (7.7), $K_1(h)$ and $C_1(h)$ are the hydraulic properties of the sand material. The effective functions of the double-porosity medium are plotted in Figs 7.7b and 7.8 respectively. Note that $K_{eff}$ calculated from the local boundary value problem corresponding to the non-equilibrium model (h2:loc7) – (h2:loc8) is outside the interval $[K_1, \ldots, K_2]$ in dry range (the model is no longer valid in this area, see Section 7.5.5). In Fig. 7.8 we also show the effective conductivity obtained from the solution of the local boundary problem associated with the local equilibrium model of Lewandowska & Laurent (2001).

### 7.4.3 Solution of the macroscopic problem

The boundary conditions at the inlet and the outlet of the column were $h_{surf} = -0.1$ mm of water at $X_3 = 0$ and $\frac{\partial h}{\partial X_3} = 0$ at $X_3 = -60$ cm. The initial condition was imposed at $h_{init} = -10$ m within the whole domain, implying initial equilibrium between the two subdomains. The calculations were made with uniform space discretization of the macroscopic domain $\Delta X = 0.5$ cm (121 nodes) as well as of the sphere domain $\Delta r = 0.016$ cm (21 nodes). The time step was allowed to vary from $10^{-6}$ s to 10 s. The accuracy was specified.
Table 7.3: Some measured and calculated flow characteristics related to the experiments performed in the column filled up with sand and the double-porosity medium. (1) mean values of Tests 1 and 2, (2) mean values of Tests 4, 5 and 6.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Sand column</th>
<th>Double-porosity column</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>measured</td>
<td>fitted</td>
</tr>
<tr>
<td>Breakthrough time [s]</td>
<td>2750</td>
<td>2500</td>
</tr>
<tr>
<td>Volumetric flux at steady state [cm s(^{-1})]</td>
<td>2.86 \times 10^{-3}</td>
<td>2.86 \times 10^{-3}</td>
</tr>
<tr>
<td>Infiltrated water at breakthrough time [cm]</td>
<td>21.1</td>
<td>20.0</td>
</tr>
<tr>
<td>Volumetric water content at steady-state regime [-]</td>
<td>0.342</td>
<td>0.342</td>
</tr>
</tbody>
</table>

in terms of pressure head. A mixed criterion with absolute tolerance of 0.1 cm of water and relative tolerance of 0.1% was used. Finer grids (\(\Delta X = 0.25\) cm and \(\Delta r = 0.0032\) cm) and smaller error tolerances were also tested but no significant influence on the results was observed. The CPU time was about 320 s for the coarser grid and 5600 s for the finer one with a Pentium IV 2.0 GHz processor.

7.5 Results and discussion

7.5.1 Comparison of the behavior of sand and double-porosity medium

The behavior of pure sand is compared to the behavior of the mixture of sand and clayey spheres to see the qualitative and quantitative influence of the inclusions. In Table 7.3 some selected “indicators” of the behavior for the two media are regrouped. As it can be seen there exists a significant difference in all these parameters, as well measured as calculated. The infiltration process lasts much longer in the double-porosity medium than in the sand column. The observed breakthrough time in double-porosity medium (5810 s) is about twice as much as in sand (2750 s), while in case of calculated values the factor is 2.8. On the other hand, the flux (measured and observed) at quasi steady-state regime (and almost saturation) is three times less in sand than in double-porosity medium. The total measured amount of water infiltrated into the column is about 16% less in case of double-
Figure 7.13: Comparison between measured and calculated infiltration fluxes in the double-porosity medium.

porosity medium than in sand. This result is confirmed by numerical simulation. We can also notice a difference between the final volumetric water contents in sand (0.342) and in the double-porosity medium (0.293 and 0.316), which can be explained by the difference in porosities between sand and sintered clayey material. The final water content measured in double-porosity medium (0.293) can be compared with its total porosity (0.316), calculated as a volume average of the porosity accessible to water in sand and clayey material. The experimental value is slightly smaller, which indicates that the porous spheres were not completely saturated (in the reduced fraction of their porosity, assumed to be accessible to water).

7.5.2 Comparison of numerical and experimental results

The comparison between the observed and simulated behavior of the double-porosity medium is presented in Figs 7.4, 7.5, 7.13 and 7.14. In Figs 7.4 and 7.5 three distinct flow phases can be observed in the cumulative infiltration curves: (i) the early infiltration, (ii) the transition phase after the beginning of discharge and (iii) the steady state flow. All these three phases seem to be well reproduced in the numerical solution. The measured and calculated
infiltration and discharge fluxes in Figs 7.13 and 7.14 seem to be in a reasonable agreement. However, in all three experiments the infiltration process was faster than in the numerical simulation. The breakthrough time is about 1200 s longer in the numerical simulation than observed. The difference cannot be attributed to the outlet boundary condition specified in the numerical solution, since this condition does not influence the solution unless the front arrives at the bottom of the column.

Another discrepancy between numerical and experimental results arises at the beginning of the outflow, Fig. 7.14. The initial discharge flux is significantly greater than the water conductivity at steady-state for $h = -0.1$ cm. It indicates the presence of a capillary pressure gradient at the bottom of the column. Such a result cannot be obtained from the numerical simulation, since free drainage (zero gradient) condition at the bottom of the column was imposed. Note that the free drainage condition is very often assumed in the column test with open outlet. This assumption seems to be justified in case of our column, as no such effect was observed in the tests with sand, which were performed in the same experimental conditions. It can partially be explained by difficult measurement conditions during the very early stage of the outflow (small values, large relative variations, poor relative measurement precision). However, since this effect was systematically observed in all three tests on mixtures, we
believe that it can be associated with the air phase flow. We think that the air pressure can not equilibrate instantaneously, as it is assumed in the model, and therefore it is not constant during the process. The lack of the peek in the discharge flux in sand can be explained by the reduced conductivity with respect to the air phase in the double-porosity as compared to the sand. We are aware of the problem but we do not have enough information to validate or reject this hypothesis. This point should be further examined.

The observed steady-state fluxes (both inlet and outlet) in the double-porosity experiments (Figs 7.13 and 7.14), corresponding to the water conductivity at \( h = -0.1 \) cm, are very close to the calculated conductivity at saturation, Table 7.3. This confirms the validity of the method of calculation of the effective water conductivity obtained by homogenization, as a solution of the local boundary value problem. It also confirms our assumption, concerning the arrangement of clayey spheres (Fig. 7.11).

### 7.5.3 Sensitivity analysis

In order to examine the sensitivity of the model with respect to the parameters of sand and clayey spheres several additional simulations were performed. In particular, the influence of the parameters \( \alpha \) and \( n \) of both media on the behavior of our model were studied. It was shown that in the case considered in this study the model is more sensitive to the parameters of sand than to the parameters of clayey spheres. In particular, it can be seen that if \( n \) is increased by 50% or \( \alpha \) decreased by 50% , the results of cumulative infiltration and breakthrough time predicted by numerical simulation are closer to the experiment Figs 7.15a and 7.15b. Nevertheless, no further attempt to obtain a better fit to the experimental data was carried out.

### 7.5.4 Exchange term and tailing effect

In Fig. 7.16a the values of the exchange term computed at selected depths in the column are presented. It can be seen that the rate of the water exchange changes very rapidly, reaches high values at the arrival of the infiltration front and diminishes also rapidly. The time of the water transfer is relatively short as compared to the breakthrough time in the column. The maximum value of the exchange rate decreases and the time of the exchange increases with time. The exchange process can be analyzed in relation with Fig. 7.16b where the profiles of the capillary pressure head at times which correspond to the maximum values of the exchange term presented in Fig. 7.16a are indicated. As it can be seen the water front is very steep during the whole process. In order to assess the importance of the exchange term for the overall water mass balance we calculated the sink term, which is the integral of
Figure 7.15: Influence of the sand parameters of the van Genuchten model on the calculated cumulative infiltration (a) and outflow flux (b) in the double-porosity medium.

exchange term defined as:

\[ \text{sink}(t) = \int_{0}^{60 \text{ cm}} Q(X,t)\,dX \]  

We compared \( \text{sink}(t) \) to the infiltration flux at the inlet of the column, Fig. 7.17. The calculations were performed for the values of infiltration flux obtained from the numerical simulation and from the experiments (we used average values from the three tests). In both cases the term \( \text{sink}(t) \) was calculated from numerical solution. In the first case this ratio varies around 0.5, during the infiltration phase up to the breakthrough. When the measured values of the infiltration flux are used, the values of \( \text{sink}(t) \) vary around 0.45. The oscillations represent the discharge of the infiltrated water towards the spheres. We can see that the amplitude of the oscillations increases with time and that the exchange process is very rapid.

In Fig. 7.18 the numerical flux at the bottom of the column in the double porosity medium (DP) is compared with the flux in the medium containing the spheres which are assumed to be impermeable (SP) and with the flux in pure sand without the inclusions. It can be concluded that the presence of inclusions in sand causes a retardation of the flux which is called tailing effect. This effect increases when the inclusions are permeable (DP case), due to the exchange process. With respect to pure sand, the inclusions cause a significant decrease in the steady-state flux.

7.5.5 Domain of validity of the model

The domain of validity of the model is defined by the ratio of the water diffusivity of the two media. This ratio is evaluated with respect to the small parameter \( \varepsilon : \frac{D_2}{D_1} = \mathcal{O}(\varepsilon^2) \). In
Figure 7.16: Time evolution of the water exchange term between sand and sintered clagey spheres calculated at different depths ($X_3$) of the column.
Chapter 7. Comparison of the theoretical model with experimental results

**Figure 7.17:** Time evolution of the ratio between the depth-integrated water exchange rate \((\text{sink}(t))\) and the observed and calculated infiltration flux \((q_0)\) in the double-porosity medium.

**Figure 7.18:** Comparison of the discharge fluxes obtained for the double-porosity (DP) medium, the single-porosity (SP) medium and the sand column.
Chapter 7. Comparison of the theoretical model with experimental results

Figure 7.19: The ratio of hydraulic conductivity ($K$), capillary capacity ($C$) and capillary diffusivity ($D$) of the clayey material (subscript 2) to the parameters of sand (subscript 1) as a function of capillary pressure head.

In our case $\varepsilon$ is equal to the ratio of the period size to the column length, $\varepsilon = 1.2 \text{ cm} / 60 \text{ cm} \approx 2 \times 10^{-2}$. In Fig. 7.19 the ratios of water conductivities, water retention capacities and water diffusivities of the two media are presented. As we can see the ratio of the diffusivities is not constant during the infiltration process and takes values ranging from $10^{-6}$ to $10^{2}$ for $h = -0.1 \text{ cm}$ and $h = -1000 \text{ cm}$, respectively. This means that our model is not valid during the whole process but only for the capillary pressure head between $h = -1 \text{ cm}$ and $h = -10 \text{ cm}$. In this range, the corresponding ratio of the diffusivities is of the order $O(10^{-5}) \ldots O(10^{-3})$ and we can conclude that the assumption $\frac{D_2}{D_1} = O(\varepsilon^2)$ is satisfied. Outside this range of $h$, either the equilibrium model for moderately heterogeneous medium (Lewandowska & Laurent, 2001) for $\frac{D_2}{D_1} = O(1)$ or the model developed for double porosity soils with highly conductive inclusions (Chapter 3, Section 3.4) for $\frac{D_2}{D_1} \geq O(\varepsilon^{-1})$, should be applied. In order to capture the effect of changing the model in the numerical solution we recommend using the model (7.4) with the effective conductivity tensor calculated according to the method presented by Lewandowska & Laurent (2001). This general approach assures
Chapter 7. Comparison of the theoretical model with experimental results

Figure 7.20: Evolution of the cumulative infiltration (a) and the discharge flux (b) according to the non-equilibrium double porosity model (DP-NEQ) and the modified model (DP-MOD), which accounts for the variability of flow conditions.

In order to evaluate the possible effect of the variable ratio of diffusivity we performed a numerical simulation with modified DPOR-1D code. The macroscopic equation has the same form as the non-equilibrium model (7.4), but the effective conductivity is calculated from the local boundary value problem (3.116)–(3.119) corresponding to the equilibrium case. Such formulation may represent various models, according to the parameter ratio. When the diffusivity in spheres is much less than in sand matrix one obtains the non-equilibrium model (7.4), since the effective conductivities calculated from (3.116)–(3.119) and (3.50)–(3.51) become equivalent. The definition of $K^{eff}$ for the equilibrium case remains valid also when the spheres are more conductive than sand (see Chapter 5). On the other hand, when the diffusivity of spheres is similar to or larger than the diffusivity of sand, the source term $Q$ can be still computed from the local flow equations. Since the pressure equilibrates very quickly, the water content becomes constant in the $\Omega_2$ sub-domain. This formulation is analogous to the equilibrium model. The results of the simulation are shown in Figs 7.20a and 7.20b. It can be seen, that the differences are not significant in our case. Thus, one can conclude that the flow is effectively governed by the local non-equilibrium model (corresponding to the wet range) and the effects associated with the dry range are not visible here.
7.5.6 Summary

The general conclusion of the study is that the model seems to be able to reproduce the characteristic features of the behavior observed in the experiments. In particular, the effective conductivity of the double porosity medium predicted by the model is in a very good agreement with the observations. Nevertheless, it is difficult to comment on the results in a definite way, since the domain of validity of the double-porosity model was not completely respected. Therefore, various effects are superposed and the double-porosity features are "hidden". Another experiment is planned in which the capillary pressure head will be kept within the "wet" zone, such that the ratio of the diffusivities satisfies the condition \( \frac{D_2}{D_1} = O(\varepsilon^2) \). Another point which needs further investigation is the assumption of the validity of the van Genuchten – Mualem model for the hydraulic functions of the two materials. In our study the hydraulic parameters of the two materials were not determined from direct measurements. They were estimated by the inverse analysis which does not guarantee the uniqueness of the solution and in which the form of the hydraulic functions has to be assumed. The future experimental program includes the direct measurements of the hydraulic functions, as well as the measurements of the water content and the capillary pressure inside the column. Another important issue to be also verified is the validity of the Richards assumption.

The non-equilibrium model presented here in its full form may be improved, if more experimental data are available. In particular, some simplifications will be necessary to make it useful from the point of view of applications in engineering practice (e.g. the approximation of water transfer term). Using the present model the simplifications can be done in a systematic and controlled way.
Chapter 8

Summary and conclusions

This study concerns the modeling of water flow in unsaturated highly heterogeneous porous media. We analyzed double-porosity soils, which are characterized by the presence of two porous sub-domains with very different hydraulic properties. The preceding chapters were focused on various aspects of modeling: theoretical, numerical and experimental. A detailed discussion of the obtained results is provided in each chapter. In this part the most important points are summarized.

The major result of the study is the derivation of the macroscopic models of flow in the double-porosity soils by the method of asymptotic homogenization (Chapter 3). We assumed that at the local scale the flow is described by the Richards equation, which is routinely used in the unsaturated zone modeling. We analyzed two different soil structures, i.e. highly conductive matrix with weakly conductive inclusions and weakly conductive matrix with highly conductive inclusions. The macroscopic behavior is described by different model for each type of medium.

In the first case a non-equilibrium flow model was obtained when the ratio of the diffusivity of the two materials is $\frac{D_2}{D_1} = \mathcal{O}(\epsilon^2)$, $\epsilon$ being the scale parameter. The resulting model has a form of a single nonlinear integro-differential equation with two macroscopic parameters (the effective capillary capacity and the effective hydraulic conductivity). The integral term describes the exchange of water between matrix and inclusions. It is obtained from the solution of the local-scale equations describing the flow in weakly conductive inclusions. Thus, the macroscopic and local variables are coupled. The effective capillary capacity depends on the capacity of the more conductive matrix and its volume fraction. The effective hydraulic conductivity depends on the conductivity of the matrix and a geometry-dependent vector function $\chi$, which is obtained from the solution of a linear local boundary value problem. Both effective parameters are linear functions of the matrix parameters. They are independent of the hydraulic characteristics of inclusions.
In the second case (i.e. soil with highly conductive inclusions, $\frac{D^2}{Dx^2} = \mathcal{O}(\varepsilon^1)$) the flow is characterized by the local equilibrium conditions. The macroscopic model has the form of a single Richards-type equation. The effective capillary capacity depends on the capacities of the two components. The effective conductivity is determined by the conductivity of the weakly conductive matrix and the local geometry. The influence of the geometry is represented by a vector function obtained from a linear local boundary value problem. The effective conductivity is independent of the conductivity of inclusions. For both considered types of geometry the effective capacity and the effective conductivity are highly nonlinear functions of the macroscopic pressure head. The two models were shown to be limit cases of the model developed by Lewandowska & Laurent (2001) for moderately heterogeneous soils.

Another aspect of this work was the numerical implementation of the mathematical models obtained from homogenization (Chapter 4). The solution of a macroscopic flow problem is performed in two stages: (i) solution of the local boundary value problem and determination of the effective parameters and (ii) simulation of macroscopic flow for specified initial and boundary conditions. In case of the non-equilibrium flow the macroscopic equation has complex form due to the presence of highly nonlinear integral source term. Thus, the macroscopic and local equations should be solved simultaneously. The coupling is treated by a specially developed numerical algorithm. The algorithm is implemented in the DPOR-1D program which has been elaborated for the purposes of this study. The macroscopic flow is assumed one-dimensional, while the local geometry can be two or three-dimensional. We used fully implicit finite difference formulation combined with Newton iterative scheme. The two- and three-dimensional local-scale flow equations are solved by the spatial decomposition method.

Calculation of the effective conductivity in double-porosity soils was studied in more detailed way in Chapter 5. We considered several types of local geometry (2D and 3D inclusions). Different factors influencing the effective conductivity were examined (the ratio of conductivity of the two components, the form, volume fraction and arrangement of inclusions). The results of calculations were compared to the theoretical bounds existing in literature. For simple isotropic geometries of inclusions (spheres, cubes, circles, squares) the effective conductivity obtained from homogenization coincides with the one obtained with Hashin & Shtrikman (1962) formula and depends mainly on the volumetric fractions of the two components. The numerical examples also showed the influence of local geometry on the anisotropy of the effective conductivity tensor.

Numerical simulations of macroscopic flow in double-porosity soils were performed for three types of local geometry (Chapter 6). The results obtained using DPOR-1D code were compared to the fine scale solution of Richards equation with explicit representation of the
Chapter 8. Summary and conclusions

heterogenous soil structure (SWMS-2D and SWMS-3D codes). In all cases the solution obtained from homogenization was close to the reference fine scale solution. The computational effort was much less for DPOR-1D simulations than for the fine scale simulations. The direct local-scale simulation of Richards equation requires very dense numerical grid in order to represent accurately the heterogeneity of the medium. When the parameters of the two sub-domains are very contrasting, additional difficulties in numerical approximation arise at the interfaces between highly and weakly conductive regions. The problems are avoided using the homogenization approach. In our tests the calculation time was at least ten times shorter for the DPOR-1D solutions than for the fine scale solutions on comparable machines.

For the non-equilibrium flow the results have been compared with phenomenologically based double-porosity model (Gerke & van Genuchten, 1993a). It has been shown that the latter model gives results close to the reference solution only for a particular, very simple geometry.

The model of non-equilibrium flow obtained by homogenization has been used to analyze the experimental results (Chapter 7). We used the results of infiltration experiments in a model double-porosity medium composed of fine sand and sintered clayey spheres arranged in periodic manner. The hydraulic properties of the two components, i.e. the sand and the sintered clayey material, were obtained from independent experiments using the inverse analysis. Those parameters were used as input data in the macroscopic model. The infiltration was simulated numerically using DPOR-1D code. The results of simulations were in good agreement with the observations. The effective hydraulic conductivity obtained from the solution of the local boundary problem for the assumed arrangement of spheres was very close to the conductivity measured in the experiments. Nevertheless, due to some shortcomings and limitations of the experimental analysis, it is difficult to draw definite conclusions. The problem would require a more comprehensive experimental program.

It can be concluded from the presented examples that the method of homogenization is an efficient approach for modeling unsaturated flow in double-porosity soils. The solutions obtained by homogenization were in good agreement with the reference fine scale numerical solutions and the experimental results. The homogenization presents an alternative to the fine scale simulations, which are usually very time-consuming and often impossible. On the other hand it has the advantage of being mathematically and physically rigorous, which distinguishes this method from routinely used phenomenological approaches.

Apart from the already mentioned experimental issues, several other aspects of this study requires further, more detailed investigation. One example concerns practical application of the local non-equilibrium flow model with the integral exchange term. The calculation of this term requires considerable numerical effort. It would be convenient to approximate the integral with a closed-form analytical expression. This would enable us to avoid tedious
solution of nonlinear local-scale flow equations in inclusions. Several propositions of such approximations can be found in literature, however their application in the considered model requires careful examination. Other possible areas of improvement of the numerical model (DPOR-1D) include extension for macroscopically two-dimensional flow or inverse problems.

Finally, one should notice that the same methodology can be used to investigate other processes in highly heterogeneous porous media. Modeling of complex phenomena as reactive multi-component contaminant transport or multi-phase flow becomes increasingly important in civil and environmental engineering. Application of the presented approach to those more complicated cases can be the subject of future research.
Résumé étendu de la thèse

Modélisation de l’écoulement d’eau dans les sols partiellement saturés et fortement hétérogènes

Introduction (Chapitre 1)

La zone non saturée des sols (ou vadose zone) est le siege à nombreux phénomènes dont l’importance n’est plus à démontrer dans de domaines tels que l’agronomie (alimentation hydrique et minérale des plantes), l’hydrologie (partition de la pluie entre infiltration et ruissellement, évapotranspiration), l’hydrogéologie (recharge des nappes), la géotechnique (stabilité des ouvrages) et l’environnement (devenir des substances chimiques, stockage des déchets). La prévision de ces phénomènes revêt une importance certaine pour le génie d’environnement et nécessite l’utilisation de modèles mathématiques aussi fiables et efficaces que possible. La difficulté de la modélisation est due à la complexité des systèmes fortement hétérogènes et à la nature fortement non linéaire des phénomènes impliqués.

Les sols (et les roches) dans la zone insaturée présentent presque toujours une structure hétérogène. Un type particulier est représenté par les milieux à double porosité. Ils sont composés de régions très perméables et de régions moins perméables, comme par exemple un sable avec des lentilles argileuses. Dans ces milieux, trois échelles d’observation peuvent être distinguées: l’échelle du pore, l’échelle locale et l’échelle macroscopique, liée aux problèmes pratiques. Puisque le nombre d’hétérogénéités peut être très grand, il est nécessaire d’utiliser des modèles macroscopiques, où le milieu hétérogène est représenté par un milieu homogène équivalent avec les paramètres effectifs. Dans les cas de milieux à double porosité, en raison du contraste entre les propriétés hydrodynamiques entre les deux systèmes poreux, l’écoulement se déroule dans les conditions de non équilibre local. Cela conduit à des modèles spécifiquement dédiés à ce type du milieu.

Ainsi la these a pour objectif principal le développement de modèles d’écoulement dans la zone insaturée à l’échelle macroscopique, à partir de la description à l’échelle locale. De
Resumé étendu de la thèse

façon plus spécifique, elle comprend trois volets:

1. le changement d’échelle micro-macro par la méthode d’homogénéisation et les développements asymptotiques;

2. la résolution numérique des équations macroscopiques ainsi obtenues et son implantation dans un code de calcul DPOR-1D, développé à cette occasion et suffisamment versatile pour simuler différentes géométries d’hétérogénéités;

3. la comparaison du modèle avec d’autres formulations proposées dans la littérature et avec des résultats expérimentaux relatifs à l’infiltration dans un milieu à double porosité constitué d’inclusions sphériques d’argile.

Etude bibliographique (Chapitre 2)

Le point de départ de notre analyse est la description mathématique de l’écoulement à l’échelle locale pour un milieu homogène. L’écoulement peut être décrit par une approche biphasique (air + eau), mais il est souvent possible de considérer la pression de la phase air comme constante et égale à la pression atmosphérique. Cette hypothèse conduit à l’équation de Richards (1931), formulée à l’aide de la variable d’état pression capillaire (Chapitre 2, Eq. 2.11). Cette équation est fortement non linéaire, puisque les paramètres (capacité capillaire et conductivité hydraulique) sont fonction de la pression capillaire. Plusieurs formulations plus ou moins empiriques ont été proposées pour exprimer les relations entre la pression capillaire \( h \), le teneur volumique en eau \( \theta \) et la conductivité \( K \). Les plus souvent utilisées sont celles de van Genuchten (1980) et Mualem (1976) ou Brooks et Corey (1964).

La description mathématique devient plus complexe à l’échelle macroscopique pour un milieu hétérogène. Deux approches différentes de la modélisation peuvent être distinguées. Dans l’approche phénoménologique, le modèle mathématique est introduit directement à l’échelle macroscopique. La forme du modèle est proposée à partir de considérations empiriques. L’autre approche (macroscopisation) consiste à dériver le modèle macroscopique à partir de la description des phénomènes à l’échelle locale. Plusieurs techniques telles que la méthode d’homogénéisation (Bensoussan et al., 1978; Sanchez-Palencia, 1980; Auriault, 1991) ou la méthode de prise de moyenne spatiale (Quintard et Whitaker, 1988; Whitaker, 1999) peuvent être utilisées.

Les différents modèles macroscopiques sont présentés dans le sous-chapitre 2.2, avec l’accent étant mis sur les milieux “classiques” à double porosité, qui sont composés d’une matrice perméable avec des inclusions plus faiblement conductrices. Cette structure particulière est à l’origine des effets du non équilibre local pendant l’écoulement. Dans l’approche


Notre étude bibliographique présente aussi les modèles d’écoulement proposés pour les autres types de milieux hétérogènes, tels que les milieux à double porosité composés d’une matrice faiblement perméable avec des inclusions très perméables (sous-chapitre 2.3.3) et les milieux faiblement hétérogènes, où les paramètres hydrodynamiques ne sont pas très contrastés (sous-chapitre 2.3.1). Finalement, nous avons aussi présenté quelques remarques sur l’implémentation numérique des modèles macroscopiques et sur les résultats expérimentaux concernant l’écoulement dans les milieux à double porosité.

L’étude bibliographique montre que la modélisation des écoulements dans les sols insaturés fortement hétérogènes est toujours un sujet d’actualité. Il apparaît que les modèles fondés sur l’approche phénoménologique sont nombreux, mais leur justification physique et mathématique peut être sujette à caution. Par contre, l’application des méthodes rigoureuses de macroscopisation est en général limitée aux problèmes d’écoulement biphasique ou saturé et ne concerne que rarement la zone insaturée.

Développement des modèles macroscopiques d’écoulement dans les sols insaturés à double porosité par la méthode d’homogénéisation (Chapitre 3)

La méthode d’homogénéisation est l’une des techniques mathématiques le plus souvent utilisée pour la modélisation des milieux hétérogènes (Hornung, 1997). Le milieu est considéré périodique et les deux échelles d’observation doivent être bien séparées, ce qui est représenté par la condition $\epsilon = l/L \ll 1$, où $\epsilon$ est un paramètre d’échelle, $l$ et $L$ sont les longueurs caractéristiques à l’échelle locale et à l’échelle macroscopique, respectivement. La séparation d’échelles permet d’introduire deux variables adimensionnelles d’espace: $x$ (variable macroscopique) et $y$ (variable locale).
Les principales étapes d’homogénéisation sont: (i) la description du phénomène physique à l’échelle locale; (ii) la normalisation des équations; (iii) l’estimation de l’ordre de grandeur des nombres adimensionnels par rapport à $\varepsilon$; (iv) l’introduction des développements asymptotiques des fonctions (Chapitre 3, Eq 3.5); (v) l’identification et la solution du problème correspondant aux puissances successives de $\varepsilon$, qui conduit à sa formulation macroscopique. La méthode est rigoureuse et ne nécessite aucune hypothèse sur la forme des équations macroscopiques. Elle permet d’obtenir les paramètres effectifs et de préciser le domaine de validité du modèle dérivé.

Le milieu considéré est composé de régions perméables $\Omega_1$ et des régions moins perméables $\Omega_2$, séparées par l’interface $\Gamma$. À l’échelle locale l’écoulement est décrit par l’équation de Richards dans chaque région. Sur l’interface entre la matrice et les inclusions la pression capillaire et le flux normal sont continus. Les caractéristiques hydriques de chaque région sont supposées connues et les fractions volumiques $w_1$ et $w_2$ de $\Omega_1$ et $\Omega_2$ respectivement sont du même ordre de grandeur.

Le premier cas de figure étudié concerne un milieu composé d’une matrice très perméable avec les inclusions faiblement perméables (Chapitre 3, Fig. 3.1a). Nous avons introduit les hypothèses suivantes: (i) le temps d’observation correspond au temps d’écoulement dans la matrice à l’échelle macroscopique, (ii) les diffusivités capillaires des deux régions sont très contrastées ($\frac{D_2}{D_1} = \mathcal{O}(\varepsilon^2)$) et (iii) à l’échelle locale, la capillarité est beaucoup plus importante que la gravité.

Un modèle macroscopique à une équation a été obtenu (Chapitre 3, Eq. 3.63). Une seule variable macroscopique est présente - la pression capillaire correspondant à la région la plus perméable. L’effet du non équilibre local est pris en compte par un terme source. Ce terme représente l’change d’eau entre les deux régions $\Omega_1$ et $\Omega_2$. Il est défini comme la variation de teneur volumique en eau moyenne dans les inclusions faiblement perméables (Chapitre 3, Eq. 3.69). Pour calculer le terme source il faut résoudre une équation d’écoulement à l’échelle locale (Chapitre 3, Eq. 3.55) dans chaque point du domaine macroscopique. Les variables macroscopiques et locales sont donc couplées.

On montre que les deux paramètres effectifs du modèle macroscopique ($C^{eff}$ et $K^{eff}$) s’expriment à l’aide de ceux de la matrice perméable et ils sont indépendants des paramètres des inclusions. La conductivité effective $K^{eff}$ (Chapitre 3, Eq. 3.68) est définie par une fonction vectoriel $\chi$ qui est obtenue par la résolution d’un problème local aux limites (Chapitre 3, Eqs 3.50 et 3.51). Elle représente l’influence de la géométrie sur la conductivité macroscopique du milieu. La capacité capillaire effective $C^{eff}$ est définie comme la capacité de la matrice multipliée par sa fraction volumique (Chapitre 3, Eq. 3.64).

Le deuxième cas étudié correspond à la configuration inverse: une matrice peu perméable
avec des inclusions très perméables (Chapitre 3, Fig. 3.1b). Ici nous avons considéré que: (i) le temps d’observation est égal au temps caractéristique de l’écoulement dans la matrice à l’échelle macroscopique, (ii) les diffusivités capillaires des deux régions sont contrastées \( (D_2/D_1 = O(\varepsilon)) \) et (iii) à l’échelle locale la capillarité est beaucoup plus importante que la gravité.

Le modèle macroscopique est une équation parabolique de type Richards (Chapitre 3, Eq. 3.110). L’écoulement se déroule dans les conditions de l’équilibre local. La conductivité effective (Chapitre 3, Eq. 3.111) est toujours définie par la fonction \( \chi \), mais le problème aux limites local est formulé de façon différente (Chapitre 3, Eqs 3.92 – 3.93). La conductivité effective dépend de la conductivité de la matrice et elle est indépendante de la conductivité des inclusions. La capacité effective est égale à la moyenne pondérée des capacités capillaires des deux composants (Chapitre 3, Eq. 3.101).

Dans la dernière partie de ce chapitre, les modèles obtenus sont comparés au modèle développé précédemment pour les milieux insaturés faiblement hétérogènes (Lewandowska et Laurent, 2001). Nous montrons que les passages entre ces modèles sont possibles. Le domaine de validité des modèles macroscopiques est présenté (Chapitre 3, Fig. 3.3).

**Implémentation numérique des modèles macroscopiques (Chapitre 4)**

Les modèles théoriques développés dans le chapitre précédent ont été implémentés dans le code DPOR-1D. Ce code permet de simuler l’écoulement 1D à l’échelle macroscopique avec des géométries locales 2D ou 3D. Plusieurs types de géométrie des inclusions sont possibles (Chapitre 4, Fig. 4.2).

Les données nécessaires pour la mise en œuvre de ces modèles sont relatives à la définition de la géométrie locale et aux caractéristiques hydriques des deux régions. La résolution est effectuée en deux étapes. D’abord il faut résoudre le problème aux limites local pour obtenir la conductivité effective du milieu. Ensuite les paramètres effectifs sont utilisés dans l’équation macroscopique, cette dernière étant résolue pour les conditions initiales et aux limites macroscopiques spécifiées. Dans le cas d’un écoulement en condition de non équilibre local l’écoulement local dans les inclusions doit être résolu conjointement.

Le problème aux limites local est décrit par une équation elliptique de type Poisson. Sa résolution est effectuée avec la méthode des différences finies (Chapitre 4, Eq. 4.11 et 4.28). La discrétisation spatiale conduit à un système d’équations algébriques linéaires avec une matrice creuse. Il est résolu par la méthode de sur-relaxation successive (sous-chapitre 4.3.3).
L’équation macroscopique présente une forme complexe. Chaque point du domaine macroscopique est en effet associé à une inclusion pour laquelle il faut résoudre l’équation d’écoulement local (Chapitre 4, Fig. 4.4). Pour sa résolution numérique, nous avons choisi la formulation mixte \((\theta - h)\) d’équation d’écoulement insaturé (Celia et al., 1990). La discrétisation spatiale est effectuée avec les différences finies (Chapitre 4, Eq. 3.39). La discrétisation par rapport au temps est effectuée selon un schéma généralisé de deuxième ordre avec un paramètre de pondération (Chapitre 4, Eq. 4.44). Pour chaque pas de temps nous avons un système d’équations non linéaires. Ils sont linéarisés par la méthode de Newton. Une attention particulière est apportée au calcul de la dérivée du terme source, qui nécessite la solution des équations d’écoulement local. Le pas de temps, variable, est ajusté automatiquement selon un algorithme fondé sur l’estimation de l’erreur de discrétisation.

Les équations de l’écoulement local présentent les formes différentes selon la structure du milieu. Elles peuvent être unidirectionnelles (coordonnées orthogonales ou radiales), bi- ou tridirectionnelles. Dans les cas 2D ou 3D nous avons appliqué une méthode de décomposition par rapport à l’espace permettant d’éviter des matrices de très grande taille. Les équations multidirectionnelles sont alors remplacées par une série d’équations unidirectionnelles.

Finalement nous avons présentés quelques informations et remarques sur la performance du code et sur le choix des paramètres numériques.

**Calcul de la conductivité effective des sols à double porosité (Chapitre 5)**

L’objectif de ce Chapitre est une analyse de la relation entre la conductivité effective du milieu à double porosité et différents facteurs tels que le rapport entre la conductivité hydraulique de deux domaines, la forme et l’arrangement des inclusions. Les calculs ont été effectués avec les inclusions plus perméables ou moins perméables que la matrice.

Tout d’abord nous avons montré que les deux problèmes aux limites locaux obtenus pour les milieux à double porosité sont les cas limites du problème aux limites local pour le milieu faiblement hétérogène (Lewandowska et Laurent, 2001). Pour une géométrie donnée, le rapport entre le conductivités effectives et cela de la matrice poreuse tend vers une valeur constant, quand le contraste des conductivités matrice - inclusions est grand \((K_1/K_2 \gg 100)\).

La relation entre la conductivité effective et la fraction volumique d’inclusions a été étudiée pour quelques formes particulières à inclusions isotropes 2D (cercles, carrés) (Chapitre 5, Fig. 5.8a et 5.9a) et 3D ( sphères, cubes) (Chapitre 5, Fig. 5.8b et 5.9b). Pour la même fraction volumique la différence entre sphères et cubes ou entre cercles et carrés apparaît négligeable. Par contre il existe une différence entre les géométries 2D et 3D. Les
résultats obtenus ont été comparés avec les bornes théoriques de Wiener (1912) et Hashin-Shtrikman (1962). Pour les inclusions faiblement perméables la conductivité effective du milieu équivalent est très proche de la borne supérieure de Hashin-Shtrikman alors que pour les inclusions très perméables elle est proche de la borne inférieure de Hashin-Shtrikman.

Une autre série de tests numériques concerne l’influence de l’arrangement spatial des inclusions sur la conductivité effective. Deux types d’inclusions ( sphères, cubes) et trois types d’arrangement ( cubique simple, cubique centré, parallélépipédique centré) ont été étudiés. Les résultats étant très voisins il semble que pour les formes simples d’inclusions la conductivité effective ne dépend que de leur fraction volumique.

Les calculs numériques ont aussi montré l’influence d’anisotropie du milieu sur la conductivité effective. L’analyse a été effectuée pour une géométrie simple 2D. Dans le cas du milieu anisotrope la méthode d’homogénéisation est particulièrement efficace, parce que toutes les caractéristiques géométriques du milieu sont prises en compte par la résolution du problème aux limites local.

**Exemples de la résolution des problèmes macroscopiques (Chapitre 6)**

Dans le Chapitre 6 nous présentons les résultats de la simulation numérique de l’infiltration dans un sol à double porosité à l’aide du code DPOR-1D. Trois types de géométrie ont été étudiés:

1. Cas A: sol à deux domaines (très perméable et faiblement perméable) connexes et continus (Chapitre 6, Fig. 6.1);

2. Cas B: sol avec des inclusions faiblement perméables dans une matrice bien perméable (Chapitre 6, Fig. 6.2); Cas A et cas B sont décrits par le même modèle macroscopique avec non équilibre local (Chapitre 3, Eq.3.63);

3. Cas C: sol avec des inclusions très permables dans une matrice peu conductrice (Chapitre 6, Fig. 6.9); Cas C est décrit par le modèle avec équilibre local (Chapitre 3, Eq. 3.110).

Les paramètres hydriques de deux régions ont été choisis de telle façon que les hypothèses concernant le rapport des diffusivités capillaires et des conductivités soient satisfaites.

Pour chaque géométrie la solution numérique a été calculée sur un maillage fin avec une représentation explicite de la structure hétérogène du milieu. Cette solution est considérée comme référence, puisque l’équation de l’écoulement est résolue à l’échelle fine, sans macroscopicisation. Pour la géométrie A et B les résultats sont comparés au modèle de Gerke et van
Genuchten (1993a) (Chapitre 6, Eqs 6.20 – 6.23) et au modèle à simple porosité (Chapitre 6, Eq 6.24), ou les inclusions sont considérées complètement imperméables. Pour la géométrie C le modèle Gerke et van Genuchten ne peut pas être appliqué et le modèle à simple porosité représente le milieu homogène sans inclusions.

Les résultats obtenus pour les cas A et B sont présentés dans les figures 6.5 – 6.8 du Chapitre 6. La solution par homogénéisation est très proche de la solution de référence. Si la solution de Gerke et van Genuchten est assez proche dans le cas A, elle apparaît très différente dans le cas B. Cela peut être expliqué par la méthode de calcul de la conductivité effective et du terme d’échange. Il est bien visible (Chapitre 6, Fig. 6.6), que l’écoulement dans le milieu à double porosité est plus lent que dans le milieu à simple porosité. Cet effet est dû au transfert d’eau de la matrice vers les inclusions faiblement perméables et conduit au phénomène bien connu de traînée (tailing effect). Pour le cas C, la solution par homogénéisation est également très proche de la solution de référence. L’analyse de la solution à l’échelle fine montre que la pression capillaire atteint l’équilibre relativement vite à l’échelle d’une période (Chapitre 6, Fig. 6.12). On observe, que l’écoulement est plus rapide à ce qui serait pour un milieu sans inclusions (Chapitre 6, Fig. 6.13).

Les solutions numériques à l’échelle fine sont relativement difficiles à obtenir, en raison du grand nombre de mailles nécessaires et au contraste des paramètres caractérisant les deux régions du milieu hétérogène. La méthode d’homogénéisation permet une réduction importante de temps de calcul. Les exemples considérés ont montré, que la solution obtenue par homogénéisation est très proche de la solution de référence.

Comparaison du modèle théorique avec les résultats expérimentaux (Chapitre 7)

Le Chapitre 7 présente la "validation" expérimentale du modèle d’écoulement de non équilibre local obtenu par la méthode de l’homogénéisation. Les expérimentations (Lewandowska et al., 2004) ont été effectuées sur un milieu à double porosité composé d’un sable fin (Hostun H38) et de billes d’argile solidifiées (6.4 mm de diamètre moyen). Les caractéristiques des deux matériaux sont présentées dans les Fig. 7.2 du Chapitre 7.

Le dispositif expérimental (Chapitre 7; Fig. 7.3) a été composé d’une colonne (60 cm de hauteur, 8 cm de diamètre) alimentée en eau par un infiltromètre à disque posé à la surface de la colonne, la pression imposée étant $h = -0.1$ cm d’eau. À la sortie de la colonne les conditions de drainage libre ont été appliquées.

Trois séries de test ont été effectuées: sur le sable homogène (Tests 1 et 2), sur le matériau argileux solidifié (Test 3) et sur le milieu à double porosité (Tests 4, 5 et 6). Tous les essais
Les deux premières séries ont eu pour but la détermination des paramètres hydrodynamiques de deux milieux pris séparément. La dernière série a été effectuée sur un mélange de sable et de billes. Pour chaque répétition (Test 4, 5 et 6) la colonne a été remplie de façon rigoureuse, afin d’assurer la périodicité du milieu. Les paramètres relatifs aux trois tests sont très proches (Chapitre 7, Tableau 7.1).

Les paramètres hydrauliques de deux matériaux ont été identifiés par la méthode inverse, la fonction coût étant exprimée par la somme des carrés des écarts entre les valeurs mesurées et calculées de l’infiltration et du drainage (Chapitre 7, Figs 7.4, 7.5, 7.9). Les relations $\theta(h)$ et $K(h)$ des deux matériaux sont représentées par les fonctionnelles de van Genuchten – Mualem (Chapitre 7, Eqs 7.1 – 7.2). Alors que 5 paramètres sont à optimiser, nous n’avons ajusté que 2 paramètres ($\alpha$ et $n$) pour le sable et 3 paramètres ($\alpha$, $n$ et $K_s$) pour l’argile, afin de limiter le problème de non unicité de la solution. Les autres paramètres ont été estimés à partir d’expérimentations ou de considérations additionnelles. Les paramètres ainsi identifiés sont présentés dans le Tableau 7.2 du Chapitre 7.

La géométrie locale a été assimilée à une période parallélépipédique avec les inclusions sphériques placées au centre et aux coins (Chapitre 7, Fig. 7.11). Pour cette géométrie, la solution du problème aux limites local fournit la relation entre la conductivité effective et la conductivité du sable (Chapitre 7, Eq. 7.6). La capacité effective est donnée par l’équation 7.7.

La simulation numérique a été effectuée avec le code DPOR-1D. Dans ce cas, les équations d’écoulement local sont 1D (inclusions sphériques). Les résultats numériques obtenus sont comparés aux résultats expérimentaux dans les Fig. 7.4, 7.5, 7.13 et 7.14. Trois phases d’écoulement peuvent être clairement distinguées: l’infiltration jusqu’à la percée, l’écoulement instationnaire après la percée et l’écoulement stationnaire. Ces trois étapes sont bien représentées par la solution numérique. Le flux calculé en régime stationnaire correspondant à la conductivité effective du milieu est très proche de la valeur mesurée.

La comparaison entre calculs et observations montre que la solution numérique tend à sous-estimer la vitesse des écoulements. Cet effet peut être lié au problème d’identification des paramètres du sable (voir les résultats de l’analyse de sensibilité, Chapitre 7, Fig. 7.15). Le deuxième effet présent dans les expérimentations est l’écoulement instationnaire après la percée dont flux est supérieur à celui du régime stationnaire. Cela indique l’existence d’un gradient de la pression capillaire à la sortie de la colonne, qui pourrait être dû à la présence d’air dans les billes.
Conclusion et perspectives (Chapitre 8)

Le principal résultat de ce travail est le développement de modèles macroscopiques d’écoulement dans des milieux poreux à double porosité en utilisant la méthode d’homogénéisation. Deux types de milieu ont été considérés. Dans le cas du milieu avec des inclusions faiblement perméables, le modèle macroscopique prend la forme d’une équation intégro-différentielle avec deux paramètres effectifs, qui dépendent des propriétés hydrodynamiques de la matrice bien perméable. Les effets de non équilibre local sont pris en compte par un terme source fortement non linéaire. Les variables macroscopiques et locales sont couplées. Le modèle dérivé pour le milieu avec les inclusions très perméables est décrit par l’équation de Richards avec des paramètres effectifs. L’écoulement se déroule dans les conditions d’équilibre local. La conductivité effective ne dépend pas de la conductivité des inclusions.

Sur le plan numérique, nous avons présenté une méthode de résolution de l’équation macroscopique intégro-différentielle, fortement non linéaire. Cette méthode a été implantée dans un code de calcul DPOR-1D. Ce dernier est actuellement opérationnel et offre la possibilité de développements ultérieurs.

Les comparaisons numériques avec la solution à l’échelle fine ont montré, que les modèles macroscopiques développés représentent le comportement du milieu hétérogène de façon correcte. Par contre le modèle phénoménologique de Gerke et van Genuchten (1993a) donne des résultats satisfaisants uniquement pour les géométries particulières. Enfin, le bon accord entre le modèle obtenu par homogénéisation et les résultats expérimentaux constitue une "validation" du calcul de propriétés effectives du milieu hétérogène, au moins pour la situation ici considérée.

Plusieurs voies de poursuite de recherche peuvent être suggérées. Par exemple, la simplification du terme source dans le modèle de non équilibre local, qui apparaît nécessaire pour la résolution de problèmes appliqués. A cet égard, la méthode d’homogénéisation peut constituer un cadre fédérateur pour analyser la pertinence des différentes approximations, qui ont été proposées dans la littérature.

La méthode présente dans cette thèse présente également un potentiel pour étudier d’autres phénomènes des transferts dans les milieux poreux fortement hétérogènes, tels que les écoulements biphasiques ou polyphasiques ou le transport de substances chimiques réactives, domaines qui devront faire l’objet de développements futurs, en liaison notamment avec les enjeux environnementaux.


Bibliography


Bibliography


Appendix A

DPOR–1D user manual

A.1 Source code

The code was divided into 9 source text files:

- auxsub.f90 auxiliary subroutines
- dpor1d.f90 main program
- globals.f90 declarations of global variables
- input.f90 reading data file
- local.f90 calculation of effective conductivity
- macsolv.f90 solution of macroscopic flow equation
- micsolv.f90 solution of flow in inclusions
- output.f90 writing output files
- soilfunc.f90 definitions of soil hydraulic functions

All files are required in the compilation process.

A.2 Creating the executable file

The executable file can be created using a Fortran 90 compiler. The detailed procedure depends on the compiler version. For example using Microsoft Visual Studio, following steps should be taken:

- choose File/New workspace
- in the Project tab of the dialog window select Fortran console application option
- input the name and location of the directory for project files (for example .../MyProjects/Dpor1d)
- copy all source files to the new created directory (e.g. using Windows Explorer)
- open all source files in Microsoft Visual Studio (File/Open...)
- compile each source file (Build/Compile)
- build executable file (Build/Build)
- if you want to run the program from the Visual Studio environment create a subdirectory test and copy your data file into this directory, then run the program (Build/Execute), the output files will appear in the subdirectory test.
• if you want to run the program independently of the Visual Studio, copy the executable version (dpor1d.exe file) from .../Dpor1d/Debug subdirectory to the directory where you want to run it, make sure you created subdirectory test with data file in the same directory, the program can be launched by double-clicking its name in Windows.

The code can be also compiled and run under Unix/Linux operating system.

### A.3 Structure of the data file

All information required by the program is stored in a single ASCII text file data.in. It can be edited by Windows Notepad or any other text editor. It should be placed in the subdirectory ***/test where *** is the directory containing the executable file dpor1d.exe. The data records are separated by comment lines, provided for better orientation when entering or changing data. The structure of file is listed below. The names of variables are written with Courier font, a short description of each variable is provided as well as its type (integer, real, etc.). The comment lines are denoted with *.

A consistent system of physical units must be consequently used for all physical parameters (e.g. cm for length and pressure head, hours for time etc.). The physical units are denoted by [L] - length, [T] - time etc. Region 1 always corresponds to the more conductive sub-domain.

* DPOR1D data file
* ProblemName

**ProblemName** text, max.12 characters, identifier placed in headings of output files

* ProblemText

**ProblemText** text, max 64 characters, short description placed in output files

*FlowType, FlowDir, Len, NNodes

**FlowType** integer number, (0, 1, 2 or 3)
0 = flow in a homogeneous medium with parameters of the region 1;
1 (with SourceType = 1 or 2) = non-equilibrium flow in a double-porosity medium, more conductive region 1 is connected and region 2 represents inclusions;
1 (with SourceType = 0) = flow in a medium with impermeable inclusions;
2 = equilibrium flow in heterogeneous medium with less conductive inclusions;
3 = flow in a medium with more conductive inclusions;

**FlowDir** real number, allowed values 0..1,
0. = horizontal flow
1. = vertical flow
intermediate values = flow in an inclined direction, the value represents sine of the inclination angle, measured with respect to the horizontal direction

**Len** real number length of the solution domain

**NNodes** integer number number of nodes, the domain will be divided into (NNodes-1) uniform intervals

*L1, L2, L3, GeomType

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L1,L2,L3  real numbers dimensions of single period in x, y and z direction (z is the direction of macroscopic flow);

GeomType  integer number, allowed values are: 1..8
1 = vertical layers
2 = vertical ”columns” of medium 1 in medium 2 (rectangular cross section)
3 = circles
4 = 2D rectangles
5 = spheres, simple arrangement
6 = 3D rectangular blocks
7 = spheres, centered arrangement
8 = 3D rect. blocks, centered arrangement

*DimA, DimB, DimC

DimA, DimB, DimC  real numbers representing dimensions of the inclusion
if GeomType = 1 only DimA is read (width of the layer of medium 2)
if GeomType = 2 only DimA and DimB are read (dimensions of the horizontal cross-section of the column)
if GeomType = 3, 5 or 7, only DimA is read (circle or sphere radius)
if GeomType = 4, only DimA and DimB are read (rectangle dimensions in the direction orthogonal and parallel to the flow, respectively)
if GeomType = 6 or 8, DimA, DimB and DimC represent block dimensions in the two direction orthogonal to the flow and the direction parallel to the flow, respectively

*N1, N2, N3

NX,NY,NZ  integer, number of nodes in each direction for the solution of flow equation in inclusions, if GeomType = 1,3,5,7 only NX is read etc. (see above)

*LocFlag, NLX, NLY, NLZ, TauSOR, OmegaSOR, Ke

LocFlag  integer number 0,1 or 2
0 = local boundary value problem is not solved, Ke is used as the value of effective coefficient (K(matrix) is multiplied by Ke)
1 = only the local boundary value problem is solved (no macroscopic solution)
2 = solution of the local problem and the macroscopic problem

NLX, NLY, NLZ  integer, numbers of nodes in each direction for the discretization of the period in the solution of local boundary value problem,

TauSOR  error tolerance for the solution of local boundary value problem, specified in terms of the residual vector norm

OmegaSOR  real number from the range (1..1.99), over-relaxation coefficient used in the solution of local boundary value problem

Ke  real number, effective conductivity coefficient, used when LocFlag = 0, if FlowType = 1 or 2 it should be equal to the ratio of the effective conductivity to the conductivity of medium 1 (Ke< 1), if FlowType = 3 it should be equal to the ratio of the effective conductivity to the conductivity of medium 2 (Ke> 1);
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*FType, Np (region 1)

**FType** integer number, hydraulic functions model for region 1
1 = tabularized functions
2 = van Genuchten-Mualem model
3 = Brooks-Corey model
4 = van Genuchten-Burdine for retention, Brooks-Corey for K(h)

**Np** number of points describing \( K(h) \) and \( \theta(h) \) curves if \( FType = 1 \)

* soil parameters

if \( FType = 1 \) enter parameters in lines, each line should correspond to one set of \( H_i, \Theta(H_i), K(H_i) \) values (max. \( i = 20 \) lines, \( H=0 \) in the first line)

if \( FType = 2 \) enter in a single line \( \ThetaS, \ThetaR, \Alpha, N, Ks \)

if \( FType = 3 \) enter in a single line \( \ThetaS, \ThetaR, \Alpha, N, Ks, \Eta \)

if \( FType = 4 \) enter in a single line

\[ \ThetaS, \ThetaR, \Alpha, N, Ks, \Eta \]

- \( \ThetaS \) saturated water content
- \( \ThetaR \) residual water content
- \( \Alpha \) parameter of the VG model or the inverse of the air entry pressure in the BC model
- \( N \) parameter of the VG model
- \( Ks \) saturated conductivity
- \( \Eta \) exponent in the BC conductivity model

*FType, Np (region 2)

Definition of the soil functions for region 2

*soil parameters (region 2)

The same structure as for region 1.

*InitType, InitValue (region 1)

**InitType** initial condition type in region 1
1 = constant value in the domain,
2 = hydrostatic distribution of pressure

**InitValue** initial pressure in the column (if \( \text{InitType}=1 \)) or initial pressure at the bottom of the column (if \( \text{InitType}=2 \))

*InitType, InitValue (region 2)

Initial condition in region 2

*BCIn, Np (top boundary)

**BCIn** boundary condition type at the top of the column
1 = specified pressure \( (h=h(t)) \)
2 = specified flux \( (q=q(t)) \)

**Np** integer, number of points describing the \( q(t) \) or \( h(t) \) function

*boundary condition points (top boundary)

Points defining the function should be entered in lines (max. 20):
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TimeI, ValueI the function is interpolated linearly between the points, if h=const or q=const, only one point should be specified (any time value can be used)

*BCOut, Np (bottom boundary)

BCOut boundary condition type at the bottom of the column
1 = specified pressure
2 = specified flux
3 = zero gradient (free drainage)

*boundary condition points (bottom) Points defining the function
*Ksi, SourceType

Ksi weighting parameter for time discretization scheme, Ksi > 0.5, (Ksi = 1. - fully implicit scheme)

SourceType method of computing the source term values
SourceType = 0 the inclusions are treated as completely impermeable and the source term is not computed and one obtains single-porosity model
SourceType = 1, the source term is computed once per time step
SourceType = 2, the source term is computed in each iteration, (recommended for highly nonlinear problems)

*DtInit, DtMin, DtMax

DtInit initial time step size [T]
DtMin minimum allowable time step size [T]
DtMax maximum allowable time step size [T]

DtMax ≥ DtInit ≥ DtMin

*NItMax, S1, S2, F1, F2

NItMax integer, maximum number of iterations in single time step
S1 real number, lower boundary of optimal error range
S2 real number, upper boundary of optimal error range, ErrOpt2 > ErrOpt1,
F1 real number, time step reduction rate, F1 < 1
F2 real number, time step increasing rate, F2 > 1

Those parameters are used in the time step control algorithm. For a more detailed description see Chapter 4.

*TauAbs, TauRel

TauAbs nonnegative real number [L] absolute error tolerance for pressure head
TauRel nonnegative real number relative error tolerance for pressure head They are used in the termination test for iteration and in time step control

*NPrint

NPrint number of print times (integer, max 20), at each print time full information on the soil profile is written

*PTimes

PTime1,....,PTimeN positive real numbers, time levels for which full profile information is written, the last number should be equal to the total simulation time

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NObs positive integer number, maximum 20, number of observation points, for which the detailed information is written at each time step, if NObs = 0 three default observation points are set at the first, central and last node of the profile

ObsZ(1),..., ObsZ(NObs) positive real numbers, the coordinates of observation nodes, the number of items in the line should be equal to NObs the numerical node closest to the specified coordinate is taken as observation point

comment line - end of data file

A.4 Output files

Several output files are created during each run. They are placed in the directory /test. They are standard ASCII text files.

datasum.out summary of the input data
runinfo.out summary of the simulation
mbalance.out information on the mass balance

T time
CQT cumulative flux at the inlet
CQB cumulative flux at the outlet
CQE cumulative exchange flux (non-equilibrium model)
WR1 total amount of water in the domain (equilibrium model) or total amount of water in the highly conductive matrix (non-equilibrium model)
WR2 total amount of water in the inclusions (non-equilibrium model)
AMBAL absolute mass balance error
AMBAL=(WR1+WR2-WR1_0-WR2_0)-(CQT-CQB)
where WR1_0 and WR2_0 are the initial amounts of water
RMBAL relative mass balance error
RMBAL=AMBAL/MAX[(WR1+WR2-WR1_0-WR2_0),(CQT-CQB)]

obsX.out evolution of the main variables at the observation points x (x = 1,...,NObs)

T time
H macroscopic water pressure head
TH macroscopic volumetric water content
K effective conductivity
Q macroscopic flux
QEX water exchange rate (non-equilibrium model)
H2 average pressure head in inclusions (non-equilibrium model)
TH2 average water content in inclusions (non-equilibrium model)
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profiles.out profiles written for each print time

Z spatial coordinate
H macroscopic water pressure head
TH macroscopic volumetric water content
K effective conductivity
Q macroscopic flux
QEX water exchange rate (non-equilibrium model)
H2 average pressure head in inclusions (non-equilibrium model)
TH2 average water content in inclusions (non-equilibrium model)

local_prof.out local pressure profiles

The profiles of local pressure in inclusions are written at each print time only for the inclusions corresponding to the observation nodes.

tlevel.out information on the numerical parameters

NB time level index
T time
DT time step
IT number of iterations
CUM IT cumulative iterations

A.5 Example

As an example we present the solution of a macroscopic problem performed with the DPOR–1D code. The problem concerns drainage of a column filled with a double porosity medium.

A.5.1 Conditions

The medium consists of sand and spheres of sintered clayey material. Both materials are characterized with the van Genuchten – Mualem functions:

\[
\begin{align*}
\theta &= \theta_r + (\theta_s - \theta_r) \left[1 + (\alpha|h|)^n\right]^{-m} \\
K &= K_s \frac{\left[1 - (\alpha|h|)^{n-1}[1 + (\alpha|h|)^n]^{-m}\right]^2}{[1 + (\alpha|h|)^n]^{m/2}}
\end{align*}
\]  

(A.1)  
(A.2)

with the following parameters:

- sand: \( K_s = 2.86 \times 10^{-3} \) cm/s, \( \theta_s = 0.342, \theta_r = 0, \alpha = 1.383 \times 10^{-2} \) 1/cm, \( n = 4.056, m = 1 - 1/n \)
- \( K_s = 1.15 \times 10^{-9} \) cm/s, \( \theta_s = 0.295, \theta_r = 0, \alpha = 6.05 \times 10^{-3} \) 1/cm, \( n = 2.27, m = 1 - 1/n \)

The spheres of radius \( R = 0.32 \) cm are arranged periodically (Fig. A.1). They are placed in the center and corners of a parallelepiped of the dimensions 0.64 x 0.64 x 1.208 cm. We assume that the column is 240 cm long. The initial condition corresponds to the full saturation — \( h_0 = 0 \) in the whole column. At the top of the column we assume an impermeable boundary (no infiltration or evaporation), while at the bottom constant pressure head \( h = 0 \) is maintained.
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A.5.2 Data file

* DPOR_1D data file (physical units (cm,h,cm/h)
* ProblemName
  Test
* ProblemText
testy numeryczne DPOR_1D
* FlowType, FlowDir, Len, NNodes
  1, 1., 240., 481
* L1, L2, L3, GeomType
  6.4d-1, 6.4d-1, 1.208d0, 7
* DimA, DimB, DimC
  3.2d-1, 0., 0.
* NX, NY, NZ
  21, 1, 1
* LocFlag, NLX, NLY, NLZ, TauSOR, OmegaSOR, Ke
  2, 65, 65, 121, 1.0d-10, 1.6, 0.
* FType, Np (region1)
  2, 0,
* soil parameters (region1)
  0.342, 0.0, 0.0138, 4.056, 2.86e-3, 3.95
* FType, Np (region2)
  2, 0,
* soil parameters (region2)
  0.295, 0.0, 0.00605, 2.269, 1.15e-9
* InitType, InitValue (region1)
  1, 0.
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* InitType, InitValue (region2)
  1, 0.
* BCIn, Np (top boundary)
  2, 1
* boundary points
  0.  0.
* BCOut, Np (bottom boundary)
  1, 1
* boundary points
  0., 0.
* Ksi, SourceType
  1., 2,
* DtInit, DtMin, DtMax
  1.e-6, 1.e-6, 10000.
* NItMax, S1, S2, F1, F2
  21, 0.66, 1., 0.8, 1.25,
* TauAbs (cm), TauRel
  0.1, 0.01
* NPtimes
  7
* PTimes
  10., 100., 1000., 1.e4, 1.e5, 1.e6, 1.e7
* NObs
  5
* ObsZ
  0., 60., 120., 180., 240.
* end of data file

A.5.3 Results

The solution of the local boundary value problem yields the following formula for the effective conductivity:

\[ K^{\text{eff}}(h) = 0.308 K_1(h) \]  \hspace{1cm} (A.3)

The profiles of water pressure head corresponding to four chosen print times are shown in Fig. A.2. The macroscopic pressure is represented by the solid lines, while the dashed lines represent the averaged pressure in the weakly conductive sub-domain at a given depth.
Figure A.2: Pressure profiles in the column.
Appendix B

DPOR–1D source code

B.1 Main program dpor1d.f90

program DPOR_1D

! Numerical code for 1D simulation of unsaturated flow in
! double-porosity soils with 2D or 3D local geometry.
! Contains procedures for calculating the effective
! parameters and solution of macroscopic problem.
! The code is based on mathematical models presented
! in the papers:
!
! Lewandowska J., Szymkiewicz A., Burzyski K., Vaucelin M.,
! Modeling of unsaturated water flow in double-porosity soils
! by the homogenization approach,
!
! Lewandowska J., Szymkiewicz A., Auriault J.-L.,
! Modeling of unsaturated water flow in soils
! with highly conductive inclusions by homogenization,
!
!----------------------------------------------------------
! declaration of modules
! each module is in separate source file with *.f90 extension
!----------------------------------------------------------

use globals
! declaration of derived types and global variables
use soilfunc
! hydraulic functions theta(h), K(h), C(h)
use local
! procedures for the solution of local boundary
! value problem and estimation of Keff(h)
use input
! procedures for reading data file
use output
! procedures for writing output files
use auxsub
! miscellaneous auxilliary procedures
use maclib
! procedures for solution of macroscopic problem
!--------------------------------------------------------
implicit none
!--------------------------------------------------------
! declarations of global variables
!--------------------------------------------------------
type (TSoilPar):: soil1,soil2

type (TMacroDis):: dmain

type (TMicroDis):: dblock

type (TLocPar):: locpar

type (TInitial):: icondf,icondb

type (TBoundary):: ubcond, lbcond

type (TNumPar):: par

type (TPrint):: ptimes

type (TMassBal):: bal

type (TRunTime):: time

!--------------------------------------------------------
real(8), allocatable:: HOld(:),HFirst(:),HNew(:),&
ThOld(:,),TNew(:,),KOld(:,),KNew(:,),&
HPrimeOld(:,),HPrimeNew(:,),HBisOld(:,),HBisNew(:,),&
ExOld(:,),ExNew(:,),FluxOld(:,),FluxNew(:,),&
HBlockOld(:,,:),HBlockNew(:,,:),&
ThBlockOld(:,,:),ThBlockNew(:,,:),&
KBlockOld(:,,:),KBlockNew(:,,:),&
HAver(:,),ThAverOld(:,),ThAverNew(:,)
real(8) KeffZ

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!------------------------------------------------------------
integer Nmain,Nblock,i,j,FlowType,err,iarray(8)
logical last_step
character(64) problemname,problemtext
character(12) cc1,cc2,cc3
!----------------------------------------------------------------
! reading data file
!-------------------------------------------------------------------
print *, 'Reading input file...
open(1,file='test/data.in',status='old')
call ReadData(1,dmain,dblock,soil1,soil2,par,icondf,icondb,ubcond,&
    lbcond,ptimes,problemname,problemtext,dmain)
close(1)
!-------------------------------------------------------------------
! opening output files
!-------------------------------------------------------------------
print *, 'Opening output files...
open(11,file='test/datasum.out')
open(12,file='test/profiles.out')
open(13,file='test/tlevel.out')
open(14,file='test/mbalance.out')
open(15,file='test/runinfo.out')
do i=11,16
    call Heading(i,problemname,problemtext)
end do
!
! initialization of variables
!
Nmain=dmain%lp
Nblock=dblock%lp
FlowType=dmain%FlowType
if (locpar%flag/=0) then
    print *,'Calculating effective conductivity...
call ComKeff(FlowType,dblock,locpar,KeffZ)
end if
select case (FlowType)
case (0)
    soil1%ke=1.
    soil1%av=1.
    soil2%av=0.
case (3)
    soil2%ke=KeffZ
    soil1%ke=KeffZ
    soil2%ke=KeffZ
    soil1%ke=KeffZ
end select
!
! writing data summary
!
call DataSum(11,dmain,dblock,soil1,soil2,icondf,icondb,ubcond,&
    lbcond,par,ptimes)
close (11)
if (locpar%flag==1) then
    print *, 'Calculation of effective parameters successfully completed...'
    stop
end if
!
!allocation of dynamic arrays
!
allocate(HOld(Nmain),stat=err)
allocate(HFirst(Nmain),stat=err)
allocate(ThOld(Nmain),stat=err)
allocate(ThNew(Nmain),stat=err)
allocate(KOld(Nmain),stat=err)
allocate(KNew(Nmain),stat=err)
allocate(HPrimeOld(Nmain),stat=err)
allocate(HPrimeNew(Nmain),stat=err)
allocate(HBisOld(Nmain),stat=err)
allocate(HBisNew(Nmain),stat=err)
allocate(FluxOld(Nmain),stat=err)
allocate(FluxNew(Nmain),stat=err)
allocate(ExOld(Nmain),stat=err)
allocate(ExNew(Nmain),stat=err)
allocate(ThAverOld(Nmain),stat=err)
allocate(ThAverNew(Nmain),stat=err)
allocate(HAver(Nmain),stat=err)
allocate(HBlockOld(Nmain,Nblock),stat=err)
allocate(HBlockNew(Nmain,Nblock),stat=err)
allocate(ThBlockOld(Nmain,Nblock),stat=err)
allocate(ThBlockNew(Nmain,Nblock),stat=err)
allocate(KBlockOld(Nmain,Nblock),stat=err)
allocate(KBlockNew(Nmain,Nblock),stat=err)
!
Appendix B. DPOR–1D source code

!initialization of parameters
!------------------------------------------------------------------
print *, 'Beginning of numerical solution...
par%t=0.
par%lastdt=par%dtinit
par%mindt=par%dtmax
par%dmaxdt=par%dmax
par%maxdt=0.
HPrimeOld=0.
HPrimeNew=0.
HBisOld=0.
HBisNew=0.
ExOld=0.
ExNew=0.
ThAverOld=0.
ThAverNew=0.
HAver=0.
call Initialization(Nmain,Nblock,HOld,ThOld,KOld,FluxOld,HBlockOld,ThBlockOld,KBlockOld,&
dmain,dblock,soil1,soil2,icondf,icondb,ubcond,lbcond,par,&
HAver,ThAverOld,ba)
call WriteLevel(13,14,par,ba)
call WriteProf(12,Nmain,HOld,ThOld,KOld,FluxOld,ExOld,HAver,ThAverOld,dmain,par%t)
do j=1,dmain%nobs
call WriteObs(j,nonum(j),Nmain,HOld,ThOld,KOld,FluxOld,ExOld,HAver,ThAverOld,dmain,par%t)
end do
!-------------------------------------------------------------------
! getting initial date and time
!--------------------------------------------------------------------
call date_and_time(cc1,cc2,cc3,iarray)
time%iyear=iarray(1)
time%imonth=iarray(2)
time%iday=iarray(3)
time%ihr=iarray(5)
time%imin=iarray(6)
time%isec=iarray(7)
!--------------------------------------------------------------------
!main loop controlled (over print time levels)
!---------------------------------------------------------------------
do i = 1,ptimes%lp
par%dt=par%lastdt
!---------------------------------------------------------------------
!inner loop controlled (over intermediate time levels)
!---------------------------------------------------------------------
do
!---------------------------------------------------------------------
! solution of equation for a single time step
!---------------------------------------------------------------------
do
! first approximation of h
if (par%ndt>2) then
HFirst=HOld+par%dt*HPrimeOld+0.5*par%dt*par%dt*HBisOld
else
HFirst=HOld
end if
HBlockNew=HBlockOld
! solution of macro problem for single time step
call MacNewton(Nmain,Nblock,HOld,HFirst,HNew,ThOld,ThNew,KOld,KNew,ExOld,ExNew,&
HBlockOld,HBlockNew,ThBlockOld,ThBlockNew,KBlockOld,KBlockNew,&
ThAverOld,ThAverNew,HAver,par,dmain,dblock,soil1,soil2,ubcond,lbcond)
! calculating derivatives dh/dt and d2h/dt2
HPrimeNew=(HNew-HOld)/par%dt
HBisNew=(hprimeNew-hprimeOld)/par%dt
! updating time step size and checking solution accuracy
call NewDt(Nmain,HOld,HNew,HPrimeOld,HPrimeNew,par,soil1,ptimes,i)
if (par%nextstep) exit
end do
!---------------------------------------------------------------------------------
! resetting of the variables after each time step and writing output
!---------------------------------------------------------------------
write (*,*) 't=',par%t
call ComFluxes(Nmain,HNew,KNew,FluxNew,dmain,par,ubcond,lbcond)
call ComBal(Nmain,ThNew,FluxOld,FluxNew,ExOld,ExNew,ba,dmain,par,dblock)
call WriteLevel(13,14,par,ba)
do j=1,dmain%nobs
call WriteObs(j,nonum(j),Nmain,HNew,ThNew,KNew,FluxNew,ExNew,HAver,ThAverNew,dmain,par%t)
end do
HOld=HNew
ThOld=ThNew
KOld=KNew
FluxOld=FluxNew
HPrimeOld=HPrimeNew
HBisOld=HBisNew
if (dmain%FlowType==1) then
HBlockOld=HBlockNew
ThBlockOld=ThBlockNew

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```
KBlockOld=KBlockNew
ExOld=ExNew
ThAverOld=ThAverNew
end if
!---------------------------------------------------------------------------------
if (par%t>=ptimes%times(i)) exit
!---------------------------------------------------------------------------------
! end of the inner loop
!---------------------------------------------------------------------
end do
!----------------------------------------------------------------------------------
! writing head/moisture profile
!---------------------------------------------------------------------
call WriteProf(12,Nmain,HNew,ThNew,KNew,FluxNew,ExNew,Haver,ThAverNew,dmain,par%t)
call WriteLocalProf(16,Nmain,NBlock,HBlockNew,dmain,dblock,par%t)
!---------------------------------------------------------------------
! end of the main loop
!---------------------------------------------------------------------
end do
!----------------------------------------------------------------------------------
! getting final date and time
!---------------------------------------------------------------------
call date_and_time(cc1,cc2,cc3,iarray)
time%year=iarray(1)
time%month=iarray(2)
time%day=iarray(3)
time%hr=iarray(4)
time%min=iarray(5)
time%sec=iarray(6)
print *, 'Simulation successfully completed...

call WriteRunInfo(15,par,bal,time)
!---------------------------------------------------------------------
! deallocating arrays
!---------------------------------------------------------------------
deallocate(HOld,stat=err)
deallocate(HFirst,stat=err)
deallocate(HNew,stat=err)
deallocate(ThOld,stat=err)
deallocate(ThNew,stat=err)
deallocate(KOld,stat=err)
deallocate(KNew,stat=err)
deallocate(HPrimeOld,stat=err)
deallocate(HPrimeNew,stat=err)
deallocate(HBisOld,stat=err)
deallocate(HBisNew,stat=err)
deallocate(FluxOld,stat=err)
deallocate(FluxNew,stat=err)
deallocate(ExOld,stat=err)
deallocate(ExNew,stat=err)
deallocate(ThAverOld,stat=err)
deallocate(ThAverNew,stat=err)
deallocate(Haver,stat=err)
deallocate(HBlockOld,stat=err)
deallocate(HBlockNew,stat=err)
deallocate(ThBlockOld,stat=err)
deallocate(ThBlockNew,stat=err)
deallocate(KBlockOld,stat=err)
deallocate(KBlockNew,stat=err)
!---------------------------------------------------------------------
! closing output files
!---------------------------------------------------------------------
do i=12,18
  close(i)
end do
do i=1,dmain%NObs
  close(nonum(i))
end do
!*****************************************************************************
end

B.2 Module globals.f90

module Globals

!contains declaration of constant parameters
!and derived data types used by DPOR–1D

implicit none

!---------------------------------------------------------
! parameters
!---------------------------------------------------------
integer, parameter:: NObMax = 10
```

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! max. number of observation nodes
character(22), parameter:: noname(10)=/'test/obs1.out ', 'test/obs2.out ','test/obs3.out ', 'test/obs4.out ',&
  'test/obs5.out ', 'test/obs6.out ','test/obs7.out ', 'test/obs8.out ',&
  'test/obs9.out ', 'test/obs10.out '/

! names of output files for observation nodes
integer, parameter:: nonum(10)=(/50,51,52,53,54,55,56,57,58,59/) ! numbers associated with output files

! for which full information (profiles) is written
integer, parameter:: NBoundMax = 20 ! max. number of points for boundary condition
real(8), parameter:: pi=3.141592654

! declarations of derived types

! geometry of macroscopic domain
real(8) Len  ! length
real(8) Dz   ! spatial interval
real(8) FlowDir ! inclination of the column
integer FlowType ! type of mathematical model
integer ObsInd(NObsMax) ! indices of observation nodes
integer Lp ! number of nodes
integer NObs ! number of observation nodes

end type TMacroDis

! geometry of microscopic domain
integer GeomType
integer lx,ly,lz,lp ! numbers of nodes in each direction
integer lx1,ly1 ! "inner" nodes for 2D problem
real(8) PerX, PerY, PerZ ! lengths
real(8) Dx,Dy,Dz ! space intervals (uniform)
real(8) PerVol,Vol1,Vol2 ! volume, surface, ratio
real(8) IncVol,IncSurf
real(8) IncSVR, IncSVRN

end type TMicroDis

! parameters for the solution of local problem
integer Flag ! control variable for local problem solution
integer NX,NY,NZ ! number of nodes in X,Y,Z direction
real(8) omega ! over-relaxation coefficient
real(8) ErrSOR ! error tolerance for SOR

end type TLocPar

! boundary conditions
integer ctype
integer lp ! number of points in table
real(8) times(NBoundMax)
real(8) values(NBoundMax)

end type TBoundary

! initial condition
integer ctype
real(8) upvalue ! value at the first node

end type TInitial

! print time levels
integer lp
Appendix B. DPOR–1D source code

! number of points
real(8) times(NPrintMax)
! print time levels
end type

type TMassBal
! mass balance
real(8) winit ! initial water content
real(8) wfin ! final water content
real(8) qin ! infiltration
real(8) qout ! drainage
real(8) qfin ! cumulative infiltration
real(8) qfout ! cumulative drainage
real(8) source ! source term
real(8) source ! cumulative source term
real(8) netq ! net flux
real(8) RelBalance ! rel. m.b. error
real(8) ABalance ! absolute m.b. error
end type

type TNumPar
! various numerical parameters
integer NIter ! nb. of iter. during time step
integer BNiter ! nb. of iter. for block solution
integer NTMax ! max. allowable nb. of iter.
integer NTiter ! cumulative nb. of iter.
integer NItMax ! max. allowable nb. of iter.
integer TIter ! cumulative nb. of iter.
integer BTiter ! cumulative nb. of iter.
integer NDt ! number of time steps
integer MinIt ! min. iter. nb.
integer MmaxIt ! max. iter. nb.
integer SourceType ! linearization of transfer term
real(8) T ! time
real(8) Dt ! time step
real(8) LastDt ! previous time step
real(8) MaxDt ! max. performed step
real(8) MinDt ! min. performed step
real(8) Beta ! time discr. par.
real(8) AbsTo1 ! abs. tolerance on dh
real(8) RelTo1 ! rel. tolerance on dh
real(8) DtInit ! initial time step
real(8) DtMin ! min. allowable time step
real(8) DtMax ! max. allowable time step
real(8) Mul1, Mul2 ! multiplier
real(8) ErrOpt1, ErrOpt2 ! multiplier
logical NextStep ! successful time step
end type

type TRunTime
! date and time of the simulation
integer(2) iyear, fyear
integer(2) imonth, fmonth
integer(2) iday, fday
integer(2) ihr, fhr
integer(2) imin, fmin
integer(2) isec, fsec
integer(2) ihun, fhun
real(8) rtime
end type

end module Globals

B.3 Module soilfunc.f90

module SoilFunc
implicit none
integer, parameter:: NPSoilMax = 20 ! max. number of points for soil function

type TSoilPar
! soil hydraulic functions
integer ftype ! 1 for tabularized functions,
  ! 2 for VanGenuchten Mualem model
  ! 3 for Brooks-Corey model
  ! 4 VanGenuchten-Burdine retention
  ! * Brooks Corey conductivity
integer lp ! number of data sets (h,theta(h),K(h)
real(8) tetas ! VGM parameter
real(8) tetar ! VGM parameter
real(8) alfa ! VGM parameter
real(8) m ! VGM parameter
real(8) n ! VGM parameter
real(8) m ! m=1-1/n (Mualem) or m=1-2/n (Burdine)
end type

end module SoilFunc
real(8) ha ! BC parameter
real(8) eta ! BC parameter
real(8) av ! volume fraction of soil material
real(8) as ! surface fraction of soil material (in cross-section)
real(8) ks ! saturated conductivity
real(8) ke ! effective coefficient (keff/k_soil)
real(8) ss ! specific storage coefficient
real(8) ph(NPSoilMax) ! tabularized pressure values
real(8) pt(NPSoilMax) ! tabularized water content values
real(8) pk(NPSoilMax) ! tabularized conductivity values
end type
contains
!***********************************************************
real(8) function FKh(h,soil)
! hydraulic conductivity as function of pressure head
implicit none
type (TSoilPar):: soil
real(8) h,f,se
integer i
select case (soil%ftype)
case (1)
! tabularized functions
if (h>=soil%ph(1)) then
  f=soil%pk(1)
else if (h<=soil%ph(soil%lp)) then
  f=soil%pk(soil%lp)
else
  do i=2,soil%lp
    if (h>soil%ph(i)) then
      f=soil%pk(i-1)+&
        (soil%pk(i)-soil%pk(i-1))*(h-soil%ph(i-1))/(soil%ph(i)-soil%ph(i-1))
      exit
    end if
  end do
end if
Fkh=f*soil%ke

case (2)
! Van Genuchten Mualem model
if (h>=0) then
  Fkh=soil%ke*soil%ks
else
  se=(1.+(soil%alfa*abs(h))**soil%n)**(-soil%m)
  Fkh=soil%ke*soil%ks*se**0.5*(1.-(1.-se**(1./soil%m))**soil%m)**2
end if

case (3)
! Brooks Corey model
if (h>=soil%ha) then
  Fkh=soil%ke*soil%ks
else
  se=(soil%alfa*abs(h))**(-soil%n)
  Fkh=soil%ke*soil%ks*se**(soil%eta)
end if

case (4)
! Van Genuchten-Burdine retention curve + Brooks Corey conductivity
if (h>=0) then
  Fkh=soil%ke*soil%ks
else
  se=(1.+(soil%alfa*abs(h))**soil%n)**(-soil%m)
  Fkh=soil%ke*soil%ks*se**soil%eta
end if
end select
end function

real(8) function FCap(h,soil)
! capillary capacity as function of pressure head
implicit none
type (TSoilPar):: soil
real(8) h,sigma,f,se
select case (soil%ftype)
case (1) ! tabularized functions
if (h>=soil%ph(1)) then
  f=soil%pk(1)
else if (h<=soil%ph(soil%lp)) then
  f=soil%pk(soil%lp)
else
  do i=2,soil%lp
    if (h>soil%ph(i)) then
      f=soil%pk(i-1)+&
        (soil%pk(i)-soil%pk(i-1))*(h-soil%ph(i-1))/(soil%ph(i)-soil%ph(i-1))
      exit
    end if
  end do
end if
FCap=f*soil%ke

!****************************************************************

case (1)
! tabularized functions
if (h>=0) then
  FCap=soil%ss
else
  sigma=1.d-4*abs(h)
  f=(FTheta(h+sigma,soil)-FTheta(h,soil))/sigma
end if
FCap=f+soil%ss

case (2,4)
! Van Genuchten Mualem model
if (h>=0) then
  FCap=soil%ss
else
  se=(1.+(soil%alfa*abs(h))**soil%n)**(-soil%m)
  f=se*soil%ss+(soil%tetas-soil%tetar)*soil%m*se
  (1.+(soil%alfa*abs(h))**soil%n)**(-soil%m-1)*soil%alfa**soil%n*abs(h)**(soil%n-1)
  FCap=f+soil%ss*se
end if

end select
end function

!*******************************************************************
real(8) function FTheta(h,soil)
! volumetric water content as function of pressure head
implicit none
type (TSoilPar):: soil
real(8) h,f
integer i
select case (soil%ftype)
case (1)
  if (h>=soil%ph(1)) then
    f=soil%pt(1)
  else if (h<=soil%ph(soil%lp)) then
    f=soil%pt(soil%lp)
  else
    do i=2,soil%lp
      if (h>soil%ph(i)) then
        f=soil%pt(i-1)+&
        (soil%pt(i)-soil%pt(i-1))*(h-soil%ph(i-1))/(soil%ph(i)-soil%ph(i-1))
        exit
      end if
    end do
  end if
  FTheta=f

case (2,4)
! Van Genuchten Mualem model
  if (h>=0.) then
    FTheta=soil%tetas
  else
    FTheta=(soil%tetar+(soil%tetas-soil%tetar)*&
    (1.+(soil%alfa*abs(h))**soil%n)**(-soil%m))
  end if

case (3)
! Brooks-Corey model
  if (h>=-soil%ha) then
    FTheta=soil%tetas
  else
    FTheta=(soil%tetar+(soil%tetas-soil%tetar)*&
    (soil%alfa*abs(h))**(-soil%n))
  end if
end select
end function

!******************************************************************
real(8) function FInvTheta(tet,soil)
! volumetric water content as function of pressure head
implicit none
type (TSoilPar):: soil
real(8) h,f
integer i
select case (soil%ftype)
case (1)
  if (h>=soil%ph(1)) then
    f=soil%pt(1)
  else if (h<soil%ph(soil%lp)) then
    f=soil%pt(soil%lp)
  else
    do i=2,soil%lp
      if (h<soil%ph(i)) then
        f=soil%pt(i-1)+&
        (soil%pt(i)-soil%pt(i-1))*(h-soil%ph(i-1))/(soil%ph(i)-soil%ph(i-1))
        exit
      end if
    end do
  end if
  FTheta=f

case (2,4)
! Van Genuchten Mualem model
  if (h>=0.) then
    FTheta=soil%tetas
  else
    FTheta=(soil%tetar+(soil%tetas-soil%tetar)*&
    (1.+(soil%alfa*abs(h))**soil%n)**(-soil%m))
  end if

case (3)
! Brooks-Corey model
  if (h>=-soil%ha) then
    FTheta=soil%tetas
  else
    FTheta=(soil%tetar+(soil%tetas-soil%tetar)*&
    (soil%alfa*abs(h))**(-soil%n))
  end if
end select
end function

!**************************************************************************
real(8) function FInvTheta(tet,soil)
Appendix B. DPOR–1D source code

! water pressure head as function of vol. water content

implicit none

real(8) tet, f, s

type (TSoilPar):: soil

integer i

select case (soil%ftype)

case (1)
! tabularized functions
if (tet>=soil%pt(1)) then
  f=soil%ph(1)
else if (tet<=soil%pt(soil%lp)) then
  f=soil%ph(soil%lp)
else
  do i=2, soil%lp
    if (tet>soil%pt(i)) then
      f=soil%ph(i-1)+&
      (soil%ph(i)-soil%ph(i-1))*(tet-soil%pt(i-1))/(soil%pt(i)-soil%pt(i-1))
      exit
    end if
  end do
end if
FInvTheta=f

case (2, 4)
! Van Genuchten Mualem model
if (tet>=soil%tetas) then
  FInvTheta=0.
else
  s=(tet-soil%tetar)/(soil%tetas-soil%tetar)
  FInvTheta=-(s**(-1./soil%m)-1.)**(1./soil%n)/soil%alfa
end if

case (3)
! Brooks-Corey model
if (tet>=soil%tetas) then
  FInvTheta=-1./soil%alfa
else
  s=(tet-soil%tetar)/(soil%tetas-soil%tetar)
  FInvTheta=-(s**(-1./soil%n))/soil%alfa
end if
end select

end function

!*****************************************************************
end module SoilFunc

B.4 Module auxsub.f90

module auxsub
! miscellaneous subroutines

use Globals
use SoilFunc

contains

!************************************************************************

subroutine Initialization(Maxeq, Maxbl, HOld, ThOld, KOld, Flux, HBlock, ThBlock, KBlock,&
  dmain, dblock, soil1, soil2, init1, init2, ubcond, lbcond, par,&
  HAver, ThAver, bal)
! assigns initial values to the nodes in macroscopic domain
! and in blocks according to specified conditions

implicit none

integer maxeq, maxbl

! use macros

type (TMacroDis):: dmain

! use data

type (TMicroDis):: dblock

! use initial

type (TInitial):: init1, init2

! use boundary

type (TBoundary):: ubcond, lbcond

! use soil

type (TSoilPar):: soil1, soil2

! use parameters

type (TNumPar):: par

! use mass balance

type (TMassBal):: bal

real(8) HOld(maxeq), ThOld(maxeq), KOld(maxeq), Flux(maxeq), &
Appendix B. DPOR–1D source code

```fortran
HBlock(maxeq,maxbl), ThBlock(maxeq,maxbl), KBlock(maxeq,maxbl), &
HAvex(maxeq), ThAvex(maxeq), ci, ci, tet_s, ph_s
integer i, j, ii, jj, kk, np, lx, ly, lxi, lyl, lyl

! setting initial values in macroscopic domain
if (init1%ctype==0) then
    HOld=FInvTheta(init1%upvalue,soil1)
else if (init1%ctype==1) then
    HOld=init1%upvalue
else
    do i=1,dmain%lp
        HOld(i)=init1%upvalue+(i-1)*dmain%dz
    end do
end if

! setting boundary values in macro. domain
if (ubcond%ctype==1) then
    HOld(1)=bvalue(0.0d0,ubcond)
end if
if (lbcond%ctype==1) then
    HOld(dmain%lp)=bvalue(0.0d0,lbcond)
end if

! calculating initial water content, fluxes and conduct. in macro
if (dmain%FlowType==3) then
    call ComK(maxeq,HOld,KOld,soil2)
else
    call ComK(maxeq,HOld,KOld,soil1)
end if
call ComFluxes(maxeq,HOld,KOld,Flux,dmain,par,ubcond,lbcond)
call ComWaterEff(maxeq,HOld,ThOld,soil1,soil2)

! setting initial values in blocks
if (dmain%FlowType==1) then
    if (init2%ctype==0) then
        HBlock=FInvTheta(init2%upvalue,soil2)
    else if (init2%ctype==1) then
        HBlock=init2%upvalue
    else
        do i=1,dmain%lp
            do j=1,dblock%lp
                HBlock(i,j)=init2%upvalue+(i-1)*dmain%dz
            end do
        end do
    end if
    if (ubcond%ctype==1) then
        HBlock(1,1:dblock%lp)=bvalue(0.0d0,ubcond)
    end if
    if (lbcond%ctype==1) then
        HBlock(dmain%lp,1:dblock%lp)=bvalue(0.0d0,lbcond)
    end if
end if

! calculation of initial water content and conductivities in blocks
do i=1,dmain%lp
    do j=1,dblock%lp
        ThBlock(i,j)=FTheta(hblock(i,j),soil2)
        Kblock(i,j)=Fkh(hblock(i,j),soil2)
    end do
    ThAver(i)=0.
    select case (dblock%geomtype)
      case (1)
        do j=1,dblock%lp-1
            ThAver(i)=ThAver(i)+0.5*(ThBlock(i,j)+ThBlock(i,j+1))*dblock%dx
        end do
        ThAver(i)=ThAver(i)/((dblock%lp-1)*dblock%dx)
      case (2)
        lx=dblock%lx
        ly=dblock%ly
        lx1=dblock%lx1
        ly1=dblock%ly1
        do ii=1,dblock%lx1-1
            do jj=1,dblock%ly1-1
                tet_s=ThBlock(i,ii+(jj-1)*lx)+&
                ThBlock(i,ii+1+(jj-1)*lx)+&
                ThBlock(i,ii+jj*lx)+&
                ThBlock(i,ii+1+jj*lx)
                ThAver(i)=ThAver(i)+0.25*tet_s*dblock%dx*dblock%dy
            end do
        end do
    end select
end do
```

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ThBlock(i,ii+jj*lx)+&
ThBlock(i,ii+1+jj*lx)
ThAver(i)=ThAver(i)+0.25*tet_s*dblock%dx*dblock%dy
end do
end do
ThAver(i)=ThAver(i)/(0.25*(dblock%PerX*dblock%PerY-dblock%IncX*dblock%IncY))

case (3)
do j=1,dblock%lp-1
  ThAver(i)=ThAver(i)+0.5*(ThBlock(i,j)+ThBlock(i,j+1))&
  *(pi*((dblock%dx*j)**2.-((dblock%dx*(j-1))))**2.))
end do
ThAver(i)=ThAver(i)/(pi*(dblock%dx*(dblock%lp-1))**2.)

case (4)
lx=dblock%X
ly=dblock%y
do ii=1,lx-1
do jj=1,ly-1
  tet_s=ThBlock(i,ii+(jj-1)*lx)+&
    ThBlock(i,ii+1+(jj-1)*lx)+&
    ThBlock(i,ii+jj*lx)+&
    ThBlock(i,ii+1+jj*lx)
  ThAver(i)=ThAver(i)+0.25*tet_s*dblock%dx*dblock%dy
end do
end do
ThAver(i)=ThAver(i)/(0.25*dblock%IncX*dblock%IncY)

case (5,7)
do j=1,dblock%lp-1
  ThAver(i)=ThAver(i)+0.5*(ThBlock(i,j)+ThBlock(i,j+1))&
  *(4./3.*pi*((dblock%dx*j)**3.-((dblock%dx*(j-1))))**3.))
end do
ThAver(i)=ThAver(i)/(4./3.*pi*(dblock%dx*(dblock%lp-1))**3.)

case (6,8)
lx=dblock%X
ly=dblock%y
lz=dblock%z
do ii=1,lx-1
do jj=1,ly-1
  do kk=1,lz-1
    np=ii+(jj-1)*lx+(kk-1)*lx*ly
    tet_s=ThBlock(i,np)&
      +ThBlock(i,np+1)&
      +ThBlock(i,np+lx)&
      +ThBlock(i,np+1+lx)&
      +ThBlock(i,np+lx*ly)&
      +ThBlock(i,np+1+lx*ly)&
      +ThBlock(i,np+1lx*1ly)
    ThAver(i)=ThAver(i)+0.125*tet_s*dblock%dx*dblock%dy*dblock%dz
end do
end do
end do
ThAver(i)=ThAver(i)/(0.125*dblock%IncVol)

end select
HAver(i)=FInvTheta(ThAver(i),soil2)
ThAver(i)=dblock%Vol2*ThAver(i)
end do
end if

! calculation of water content integral
! initialization of mass balance
Bal%winit=0.
do i=1,dmain%lp-1
  bal%winit=bal%winit+0.5*(ThOld(i)+ThOld(i+1))*dmain%dz
bal%winit=bal%winit+0.5*(ThAver(i)+ThAver(i+1))*dmain%dz
end do
bal%wfin=bal%winit
bal%wbfin=bal%winit
bal%qin=0.
bal%qout=0.
bal%tsource=0.
bal%netq=0.
bal%abalance=0.
bal%relbalance=0.
end subroutine Initialization

**************************************************************************
subroutine NewDt(Maxeq,h0,h1,hprime0,hprime1,par,soil,ptimes,i)
!
!
!
end subroutine newdt

real(8) function LinInter(x0,lp,tx,ty)
!

integer lp,i
real(8) x0,tx(lp),ty(lp),f

if (x0<tx(1)) then
  f=ty(1)
else if (x0>tx(lp)) then
  f=ty(lp)
else
  do i=2,lp
    if (x0<tx(i)) then
      f=ty(i-1)+(ty(i)-ty(i-1))*(x0-tx(i-1))/(tx(i)-tx(i-1))
      exit
    end if
  end do
end if

LinInter=f

end function

real(8) function BValue(t,con)
!
!
!
end function

subroutine ComFluxes(maxeq,h,kk,qq,dmain,par,ubcond,lbcond)
Appendix B. DPOR–1D source code

! calculates fluxes
! 1st order approximation for boundary nodes
! 2nd order approximation for inner nodes

implicit none

integer maxeq,i,lp

! type(TMacrotDis) :: dmain
! type(TNumPar) :: par
! type(TBoundary) :: ubcond, lbcond

real(8) h(maxeq), kk(maxeq), qq(maxeq), k1, k2, q1, q2, cin

cin = dmain%FlowDir
lp = dmain%lp

k1 = 0.5*(kk(1):kk(2))
qq(1) = k1*(h(2)-h(1))/dmain%dz + cin*k1

do i = 2, lp-1
  k2 = 0.5*(kk(i)+kk(i+1))
  q2 = k2*(h(i+1)-h(i))/dmain%dz + cin*k2
  qq(i) = 0.5*(q1+q2)
  q1 = q2
end do

qq(lp) = q2

if (ubcond%ctype==2) then
  qq(1) = 0.5*qq(1) + 0.5*bvalue(par%t, ubcond)
  ! qq(1) = bvalue(par%t, ubcond)
end if

if (lbcond%ctype==2) then
  qq(lp) = 0.5*qq(lp) + 0.5*bvalue(par%t, lbcond)
  ! qq(lp) = bvalue(par%t, lbcond)
else if (lbcond%ctype==3) then
  ! qq(lp) = -kk(lp-1)*(h(lp)-h(lp-2))/2./dmain%dz + cin*kk(lp-1)
  ! qq(lp) = 0.5*qq(lp) + 0.5*qq(lp-1)
  qq(lp) = kk(lp)*cin
end if

end subroutine ComFluxes

!****************************************************************

subroutine ComWater(lp, h, theta, soil)
! calculates water content from pressure head
implicit none

integer i, lp
real(8) h(lp), theta(lp)
type(TSoilPar) :: soil

do i = 1, lp
  theta(i) = FTheta(h(i), soil)
end do

end subroutine ComWater

!*****************************************************************

subroutine ComWaterEff(lp, h, theta, soil1, soil2)
! calculates average water content from pressure head
implicit none

integer i, lp
real(8) h(lp), theta(lp)
type(TSoilPar) :: soil1, soil2

do i = 1, lp
  theta(i) = soil1%av*FTheta(h(i), soil1) + soil2%av*FTheta(h(i), soil2)
end do

end subroutine ComWaterEff

!*****************************************************************

subroutine ComK(lp, h, kk, soil)
! calculates hydraulic conductivity from pressure head
implicit none

integer i, lp
real(8) h(lp), kk(lp)
type(TSoilPar) :: soil

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```fortran
do i=1,lp
    kk(i)=FKh(h(i),soil)
end do

end subroutine ComK

!*****************************************************************
subroutine ComMBal(maxeq,th,qq0,qq,sq0,sq,thaver,bal,dmain,par,dblock)
! calculates mass balance
implicit none
integer maxeq,j
real(8) th(maxeq),qq0(maxeq),qq(maxeq),sq0(maxeq),sq(maxeq),&
    thaver(maxeq), counter,denom,aa,bb
type(TMacroDis):: dmain
type(TMassBal):: bal
type(TNumPar):: par
type (TMicroDis):: dblock
bb=par%beta
aa=1.-par%beta
! numerical approximation of inflow
bal%qin=(aa*qq0(1)+bb*qq(1))*par%LastDt
! numerical approximation of outflow
bal%qout=(aa*qq0(dmain%lp)+bb*qq(dmain%lp))*par%LastDt
! cumulative fluxes
bal%tqin=bal%tqin+bal%qin
bal%tqout=bal%tqout+bal%qout
bal%wfin=0.
bal%wbfin=0.
bal%source=0.
do j=1,dmain%lp-1
    bal%wfin=bal%wfin+0.5*(th(j)+th(j+1))*dmain%dz
end do
do j=1,dmain%lp-1
    bal%wbfin=bal%wbfin+0.5*(thaver(j)+thaver(j+1))*dmain%dz
end do
do j=1,dmain%lp-1
    bal%source=bal%source+aa*0.5*(sq0(j)+sq0(j+1))*dmain%dz
end do
do j=1,dmain%lp-1
    bal%source=bal%source+bb*0.5*(sq(j)+sq(j+1))*dmain%dz
end do
bal%TSource=bal%TSource+bal%source*par%lastdt
bal%netq=bal%tqin-bal%tqout+bal%tsource
bal%ABalance=abs(bal%wfin-bal%winit-bal%netq)
denom=max(abs(bal%wfin-bal%winit),abs(bal%netq))
if (denom/=0.0d0) then
    bal%RelBalance=bal%ABalance/denom*100.
else
    bal%RelBalance=0.
end if
end subroutine ComMBal

!*****************************************************************
subroutine Termin(lr,tab1,tab2,epsa,epsr,endcalc)
! checks for termination of iterations
implicit none
integer i,lr
real(8) epsa,epsr,tab1(lr),tab2(lr),error(lr),difmax
logical endcalc
endcalc=.true.
error=epsa+epsr*min(abs(tab1),abs(tab2))
difmax=minval(error-abs(tab2-tab1))
if (difmax<0) endcalc=.false.
end subroutine Termin

!*****************************************************************
subroutine Thomas(lr,a,b,c,v,x)
```
Appendix B. DPOR–1D source code

! solves linear system with tridiagonal coefficient matrix
! by the Thomas algorithm

implicit none
integer lr
real(8) a(lr), b(lr), c(lr), w(lr)
! lower diagonal, upper diagonal, main diagonal, right hand side vector
real(8) x(lr)
! solution
real(8) a1(lr), b1(lr)
integer i
real(8) p
a1(2)=-b(1)/c(1)
b1(2)=w(1)/c(1)
do i=2, lr-1
  p=(c(i)+a(i)*a1(i))
a1(i+1)=-b(i)/p
  b1(i+1)=(w(i)-a(i)*b1(i))/p
end do
x(lr)=(w(lr)-a(lr)*b1(lr))/(c(lr)+a(lr)*a1(lr))
do i=1, lr-1
  x(lr-i)=a1(lr-i+1)*x(lr-i+1)+b1(lr-i+1)
end do
end subroutine Thomas

!********************************************************************
end module auxsub

B.5 Module local.f90

module local
use Globals
! variables and subroutines for the solution of local problem
implicit none
real(8), allocatable:: a(:,:)
real(8), allocatable:: b(:)
real(8), allocatable:: q(:)
real(8), allocatable:: xx(:),yy(:),zz(:)
integer, allocatable:: ita(:,:)
integer, allocatable:: lne(:)
integer, allocatable:: mat(:)
integer, allocatable:: mat1(:,::)
contains
!**********************************
real(8) function kf(i)
implicit none
integer i
if (mat(i)==1) then
  kf=1.0d0
else
  kf=1.0d-12
end if
end function
!*********************************
subroutine sor(Neq,Sigma,Omega)
implicit none
! error tolerance
real(8) s,r,rr,sigma,omega
integer i,j,k,neq
k=0
do 
  rr=0.
do i=1,neq
    s=0.
do j=1,lne(i)

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Appendix B. DPOR–1D source code

```fortran
s = s + q(ita(i,j))*a(i,j)
end do
r = (b(i) - s)/a(i,1)
q(i) = q(i) + Omega*r
end do
rr = sqrt(rr)/neq
k = k + 1
print *, k, rr
if (rr <= Sigma) exit
end do
end subroutine sor

!************************************
subroutine Coefficients(FlowType, FlowDir, Nx, Ny, Nz, Dx, Dy, Dz)
! building coefficient matrix
! for qx, qy i qz
implicit none
integer FlowType, FlowDir, i, j, k, np, index, nx, ny, nz
real(8) kx1, kx2, ky1, ky2, kz1, kz2, cx, cy, cz
real(8) dx, dy, dz
! initialization
a = 0.
b = 0.
q = 0.
ita = 0
lne = 0
cx = 1./dx/dx
cy = 1./dy/dy
cz = 1./dz/dz
! loop over all nodes
do i = 1, nx
  do j = 1, ny
    do k = 1, nz
      ! number of node in global numeration
      np = (k-1)*nx*ny+(j-1)*nx+i
      ! coefficient at main diagonal
      ita(np,1)=np
      index = 1
      !-----------------------------------
      ! x=0
      if (i == 1) then
        kx2 = max(kf(np), kf(np+1))
a(np,1) = 2.*cx*kx2
        index = index + 1
        a(np,index) = -2.*cx*kx2
        ita(np,index) = np + 1
      ! x=L
      else if (i == nx) then
        kx1 = max(kf(np), kf(np-1))
a(np,1) = 2.*cx*kx1
        index = index + 1
        a(np,index) = -2.*cx*kx1
        ita(np,index) = np - 1
      ! x inner nodes
      else
        kx1 = max(kf(np), kf(np-1))
kx2 = max(kf(np), kf(np+1))
a(np,1) = cx*(kx1+kx2)
        index = index + 1
        a(np,index) = -cx*kx1
        ita(np,index) = np - 1
        index = index + 1
        a(np,index) = -cx*kx2
        ita(np,index) = np + 1
        if (Flowdir == 1) b(np) = kx2/dx-kx1/dx
    end do
  end do
end do
end subroutine Coefficients
```

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end if

!----------------------------------
! y=0
if (j==1) then
  ky2=max(kf(np),kf(np+nx))
a(np,1)=a(np,1)+2.*cy*ky2
index=index+1
a(np,index)=-2.*cy*ky2
ita(np,index)=np+nx
! y=L
else if (j==ny) then
  ky1=max(kf(np),kf(np-nx))
a(np,1)=a(np,1)+2.*cy*ky1
index=index+1
a(np,index)=-2.*cy*ky1
ita(np,index)=np-nx
! y inner nodes
else
  ky1=max(kf(np),kf(np-nx))
  ky2=max(kf(np),kf(np+nx))
a(np,1)=a(np,1)+cy*(ky1+ky2)
index=index+1
a(np,index)=-cy*ky1
ita(np,index)=np-nx
index=index+1
a(np,index)=-cy*ky2
ita(np,index)=np+nx
if (Flowdir==2) b(np)=ky2/dy-ky1/dy
end if

!----------------------------------
! z=0
if (k==1) then
  kz2=max(kf(np),kf(np+nx*ny))
a(np,1)=a(np,1)+2.*cz*kz2
index=index+1
a(np,index)=-2.*cz*kz2
ita(np,index)=np+nx*ny
! z=L
else if (k==nz) then
  kz1=max(kf(np),kf(np-nx*ny))
a(np,1)=a(np,1)+2.*cz*kz1
index=index+1
a(np,index)=-2.*cz*kz1
ita(np,index)=np-nx*ny
! z inner nodes
else
  kz1=max(kf(np),kf(np-nx*ny))
  kz2=max(kf(np),kf(np+nx*ny))
a(np,1)=a(np,1)+cz*(kz1+kz2)
index=index+1
a(np,index)=-cz*kz1
ita(np,index)=np-nx*ny
index=index+1
a(np,index)=-cz*kz2
ita(np,index)=np+nx*ny
if (Flowdir==3) b(np)=kz2/dz-kz1/dz
end if

!----------------------------------
! nle(np)=index
end do
end do
end do
Appendix B. DPOR–1D source code

! boundary condition qx=0 for x=0 and x=L

select case (FlowDir)
case (1)
do j=1,ny
do k=1,nz
! brzeg x=0
np=(j-1)*nx+(k-1)*ny*nx+1
a(np,1)=1.
lne(np)=1
ita(np,1)=np
! brzeg x=L
np=np+nx-1
a(np,1)=1.
lne(np)=1
ita(np,1)=np
end do
doi do
if (FlowType==3) then
do i=1,nx*ny*nz
if (mat(i)==2) then
a(i,1)=1.
lne(i)=1
ita(i,1)=i
b(i)=xx(i)
q(i)=xx(i)
end if
end do
end if
end if

! boundary condition qy=0 for y=0 and y=L
case (2)
do i=1,nx
do k=1,nz
! brzeg y=0
np=i+(k-1)*ny*nx
a(np,1)=1.
lne(np)=1
ita(np,1)=np
! brzeg y=L
np=np+(ny-1)*nx
a(np,1)=1.
lne(np)=1
ita(np,1)=np
end do
doi do
if (FlowType==3) then
do i=1,nx*ny*nz
if (mat(i)==2) then
a(i,1)=1.
lne(i)=1
ita(i,1)=i
b(i)=yy(i)
q(i)=yy(i)
end if
end do
end if
end if

! boundary condition qz=0 for z=0 and z=L
case (3)
do i=1,nx
do j=1,ny
! brzeg z=0
np=(j-1)*nx+i
a(np,1)=1.
Appendix B. DPOR–1D source code

lne(np)=1
ita(np,1)=np
! brzeg z=L
np=np+(nz-1)*nx*ny
a(np,1)=1.
lne(np)=1
ita(np,1)=np
end do
end do
if (FlowType==3) then
  do i=1,nx*ny*nz
    if (mat(i)==2) then
      a(i,1)=1.
lne(i)=1
ita(i,1)=i
b(i)=zz(i)
q(i)=zz(i)
    end if
  end do
end if
end select
end subroutine Coefficients

!********************************************************
subroutine GradVol(FlowDir,Keff,Nx,Ny,Nz,Dx,Dy,Dz)
implicit none
integer FlowDir,i,j,k,np1,np2,np3,np4,np5,np6,np7,np8
integer Nx,Ny,Nz
real(8) grad1,grad2,grad3,grad4,vg,dv,km,ind,keff
real(8) dx,dy,dz,v
v=0.
dv=dx*dy*dz
vg=0.
do i=1,nx-1
  do j=1,ny-1
    do k=1,nz-1
      np1=i+(j-1)*nx+(k-1)*nx*ny
      np2=np1+nx
      np3=np1+nx*ny
      np4=np1+nx*ny*nx
      np5=np1+1
      np6=np2+1
      np7=np3+1
      np8=np4+1
      if (mat1(i,j,k)==1) then
        km=1.0d0
      else
        km=1.0d-13
      end if
      select case (flowdir)
        case (1)
          grad1=km*(q(np5)-q(np1))/dx+km
          grad2=km*(q(np6)-q(np2))/dx+km
          grad3=km*(q(np7)-q(np3))/dx+km
          grad4=km*(q(np8)-q(np4))/dx+km
          vg=vg+0.25*(grad1+grad2+grad3+grad4)*dv
        case (2)
          grad1=km*(q(np2)-q(np1))/dy+km
          grad2=km*(q(np6)-q(np2))/dy+km
          grad3=km*(q(np7)-q(np3))/dy+km
          grad4=km*(q(np8)-q(np4))/dy+km
          vg=vg+0.25*(grad1+grad2+grad3+grad4)*dv
        case (3)
          grad1=km*(q(np3)-q(np1))/dz+km
          grad2=km*(q(np6)-q(np2))/dz+km
          grad3=km*(q(np7)-q(np3))/dz+km
          grad4=km*(q(np8)-q(np4))/dz+km
          vg=vg+0.25*(grad1+grad2+grad3+grad4)*dv
      end select
    v=v+dv
  end do
end do
end subroutine GradVol
Appendix B. DPOR–1D source code

keff=vg/v
end subroutine GradVol

!***********************************************************************
subroutine GradSurf(FlowDir,Keff,Nx,Ny,Nz,Dx,Dy,Dz)
implicit none
integer FlowDir,i,j,k,np1,np2,np3,np4,np5,np6,np7,np8,np9
integer Nx,Ny,Nz
real(8) grad1,grad2,grad3,grad4,s,v1,ds,km,ind,cc,sgrad,keff
real(8) Dx,Dy,Dz

select case (FlowDir)
case (1)
ds=dy*dz
s=0.
sgrad=0.
do j=1,Ny-1
   do k=1,Nz-1
      np1=j*nx+(k-1)*nx*ny
      np2=np1-1
      grad1=(q(np1)-q(np2))/dx+1.
      np3=np1+nx
      np4=np3-1
      grad2=(q(np3)-q(np4))/dx+1.
      np5=np1+nx*ny
      np6=np5-1
      grad3=(q(np5)-q(np6))/dx+1.
      np7=np1+nx*ny+nx
      np8=np7-1
      grad4=(q(np7)-q(np8))/dx+1.
      sgrad=sgrad+0.25*(grad1+grad2+grad3+grad4)*ds
      s=s+ds
   end do
end do
keff=sgrad/s

case (2)
ds=dx*dz
s=0.
sgrad=0.
do i=1,Nx-1
   do k=1,Nz-1
      np1=(Ny-1)*nx+i+(k-1)*nx*ny
      np2=np1-nx
      grad1=(q(np1)-q(np2))/dy+1.
      np3=np1+nx
      np4=np3-1
      grad2=(q(np3)-q(np4))/dy+1.
      np5=np1+nx*ny
      np6=np5-1
      grad3=(q(np5)-q(np6))/dy+1.
      np7=np1+nx*ny+nx
      np8=np7-1
      grad4=(q(np7)-q(np8))/dy+1.
      sgrad=sgrad+0.25*(grad1+grad2+grad3+grad4)*ds
      s=s+ds
   end do
end do
keff=sgrad/s

case (3)
ds=dx*dy
s=0.
sgrad=0.
do i=1,Nx-1
   do j=1,Ny-1
      np1=(nx-1)*nx*ny+(j-1)*nx+i
      np2=np1-nx*ny
      grad1=(q(np1)-q(np2))/dz+1.
      np3=np1+1
      np4=np3-nx
      grad2=(q(np3)-q(np4))/dz+1.
      np5=np1+nx*ny+1
      np6=np5-nx
      grad3=(q(np5)-q(np6))/dz+1.
      np7=np1+nx*ny
      np8=np7-nx
      grad4=(q(np7)-q(np8))/dz+1.
      sgrad=sgrad+0.25*(grad1+grad2+grad3+grad4)*ds
      s=s+ds
   end do
end do
keff=sgrad/s
end subroutine GradSurf

np5=np1+nx
np6=np6-nx*ny
grad3=-(q(np5)-q(np6))/dz+1.
np7=np1+nx+1
np8=np7-nx*ny
grad4=-(q(np7)-q(np8))/dz+1.
sgrad=sgrad+0.25*(grad1+grad2+grad3+grad4)*ds
g=s+ds
do end do keff=sgrad/s
do end select

end subroutine GradSurf

!********************************************
subroutine ComKeff(FlowType,dblock,LocPar,KeffZ)
implicit none
type(TMicroDis) dblock
type(TLocPar) LocPar
real(8) ax,ay,az,ar,ah,x0,y0,z0,x,y,z
real(8) x1,y1,z1,KeffX,KeffY,KeffZ,dx,dy,dz
real(8) CentX(9),CentY(9),CentZ(9),xpl,yp2,zp2,yp3,zp3
integer i,j,k,ii,err,np,inum,isph
integer neq,nx,ny,nz,FlowType,FlowDir
KeffX=0.
KeffY=0.
KeffZ=0.
FlowDir=3
select case (dblock%GeomType)
case (1,2)
KeffZ=dblock%Vol1
goto 99
case (3,4)
 nx=LocPar%NX
 ny=LocPar%NY
 nz=LocPar%NZ
 dx=dblock%PerX/(nx-1)
 dy=dblock%PerZ/(ny-1)
 dz=dblock%PerY/(nz-1)
case (5,6,7,8)
 nx=LocPar%NX
 ny=LocPar%NY
 nz=LocPar%NZ
 dx=dblock%PerX/(nx-1)
 dy=dblock%PerZ/(ny-1)
 dz=dblock%PerY/(nz-1)
end select
neq=nx*ny*nz
allocate(a(neq,7),stat=err)
allocate(ita(neq,7),stat=err)
allocate(lne(neq),stat=err)
allocate(b(neq),stat=err)
allocate(q(neq),stat=err)
allocate(mat(neq),stat=err)
mat=1
allocate(mat1(nx,ny,nz),stat=err)
mat1=1
if (FlowType==3) then
allocate(xx(neq),stat=err)
allocate(yy(neq),stat=err)
allocate(zz(neq),stat=err)
do i=1,nx
do j=1,ny
do k=1,nz
Appendix B. DPOR–1D source code

```
np=i+(j-1)*nx+(k-1)*nx*ny
xx(np)=(i-1)*dx-0.5*dblock%PerX
yy(np)=(j-1)*dy-0.5*dblock%PerY
zz(np)=(k-1)*dz-0.5*dblock%PerZ
end do
end do
end do
end if

! setting material distribution in solution domain
select case (dblock%GeomType)
case (3) !cylinder
FlowDir=2
x0=0.5*dblock%PerX
y0=0.5*dblock%PerY
ar=dblock%IncX
do i=1,nx
  x=(i-1)*dx
  x1=x+0.5*dx
  do j=1,ny
    y=(j-1)*dy
    y1=y+0.5*dy
    do k=1,nz
      np=i+(j-1)*nx+(k-1)*nx*ny
      if ((x-x0)**2.+(y-y0)**2.<=ar*ar) then
        mat(np)=2
      end if
      if ((x1-x0)**2.+(y1-y0)**2.<=ar*ar) then
        mat1(i,j,k)=2
      end if
    end do
  end do
end do
case (4) ! rectangle
FlowDir=2
x0=0.5*(dblock%PerX-dblock%IncX)
y0=0.5*(dblock%PerY-dblock%IncY)
ar=dblock%IncX
dblk%IncY
ax=dblock%IncX
ay=dblock%IncY
do i=1,nx
  x=(i-1)*dx
  x1=x+0.5*dx
  do j=1,ny
    y=(j-1)*dy
    y1=y+0.5*dy
    do k=1,nz
      z=(k-1)*dz
      z1=z+0.5*dz
      np=i+(j-1)*nx+(k-1)*nx*ny
      if ((x>=x0).and.(x<=x0+ax).and.(y>=y0).and.(y<=y0+ay)) then
        mat(np)=2
      end if
      if ((x1>=x0).and.(x1<=x0+ax).and.(y1>=y0).and.(y1<=y0+ay)) then
        mat1(i,j,k)=2
      end if
    end do
  end do
end do
case (5) ! spheres
x0=0.5*dblock%PerX
y0=0.5*dblock%PerY
z0=0.5*dblock%PerZ
ar=dblock%IncX
ax=dblock%IncX
do i=1,nx
  x=(i-1)*dx
  x1=x+0.5*dx
  do j=1,ny
    y=(j-1)*dy
    y1=y+0.5*dy
    do k=1,nz
      z=(k-1)*dz
      z1=z+0.5*dz
      np=i+(j-1)*nx+(k-1)*nx*ny
      if (((x-x0)**2.+(y-y0)**2.+(z-z0)**2.)<=ar*ar) then
        mat(np)=2
      end if
      if (((x1-x0)**2.+(y1-y0)**2.+(z1-z0)**2.)<=ar*ar) then
        mat1(i,j,k)=2
      end if
    end do
  end do
end do
```

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end if
end do
end do
end do
case (6) !parallelepiped
x0=0.5*(dblock%PerX-dblock%IncX)
y0=0.5*(dblock%PerY-dblock%IncY)
z0=0.5*(dblock%PerZ-dblock%IncZ)
ax=dblock%IncX
ay=dblock%IncY
az=dblock%IncZ
do i=1,nx
 x=(i-1)*dx
 x1=x+0.5*dx
do j=1,ny
 y=(j-1)*dy
 y1=y+0.5*dy
do k=1,nz
 z=(k-1)*dz
 z1=z+0.5*dz
 np=i+(j-1)*nx+(k-1)*nx*ny
 if ((x>=x0).and.(x<=x0+ax).and.&
  (y>=y0).and.(y<=y0+ay).and.&
  (z>=z0).and.(z<=z0+az)) then
  mat(np)=2
 end if
if ((x1>=x0).and.(x1<=x0+ax).and.&
  (y1>=y0).and.(y1<=y0+ay).and.&
  (z1>=z0).and.(z1<=z0+az)) then
  mat1(i,j,k)=2
 end if
end do
end do
end do
case (7) !centered spheres
xp1=dblock%PerX
xp2=0.5*dblock%PerX
yp1=dblock%PerY
yp2=0.5*dblock%PerY
zp1=dblock%PerZ
zp2=0.5*dblock%PerZ
CentX=(/0.0d0,0.0d0,xp1,xp1,xp2,0.0d0,0.0d0,xp1,xp1/)
CentY=(/0.0d0,yp1,0.0d0,yp1,yp2,0.0d0,yp1,0.0d0,yp1/) ar=dblock%IncX
do isph=1,9
 x0=CentX(isph)
y0=CentY(isph)
z0=CentZ(isph)
do i=1,nx
 x=(i-1)*dx
 x1=x+0.5*dx
do j=1,ny
 y=(j-1)*dy
 y1=y+0.5*dy
do k=1,nz
 z=(k-1)*dz
 z1=z+0.5*dz
 if (((x-x0)**2.+(y-y0)**2.+(z-z0)**2.)<=ar*ar) then
  mat(np)=2
 end if
if (((x1-x0)**2.+(y1-y0)**2.+(z1-z0)**2.)<=ar*ar) then
  mat1(i,j,k)=2
 end if
end do
end do
end do
case (8) !centered parallelepipeds
xp1=dblock%PerX-0.5*dblock%IncX
xp2=-0.5*dblock%IncX
xp3=0.5*(dblock%PerX-dblock%IncX)
yp1=dblock%PerY-0.5*dblock%IncY
yp2=-0.5*dblock%IncY
yp3=0.5*(dblock%PerY-dblock%IncY)
zp1=dblock%PerZ-0.5*dblock%IncZ
zp2=-0.5*dblock%IncZ
zp3=0.5*(dblock%PerZ-dblock%IncZ)
Appendix B. DPOR–1D source code

CentX=(/xp1,xp1,xp1,xp1,xp2,xp2,xp2,xp2,xp3/)  
CentY=(/yp1,yp1,yp2,yp2,yp1,yp1,yp2,yp2,yp3/)  
CentZ=(/zp1,zp2,zp1,zp2,zp1,zp2,zp1,zp2,zp3/)  
ax=dblock%IncX  
ay=dblock%IncY  
az=dblock%IncZ  
do isph=1,9  
x0=CentX(isph)  
y0=CentY(isph)  
z0=CentZ(isph)  
do i=1,nx  
x=(i-1)*dx  
x1=x+0.5*dx  
do j=1,ny  
y=(j-1)*dy  
y1=y+0.5*dy  
do k=1,nz  
z=(k-1)*dz  
z1=z+0.5*dz  
np=i+j+k  
if ((x>=x0).and.(x<=x0+ax).and.&  
     (y>=y0).and.(y<=y0+ay).and.&  
     (z>=z0).and.(z<=z0+az)) then  
  mat(np)=2  
end if  
if ((x1>=x0).and.(x1<=x0+ax).and.&  
     (y1>=y0).and.(y1<=y0+ay).and.&  
     (z1>=z0).and.(z1<=z0+az)) then  
  mat1(i,j,k)=2  
end if  
end do  
end do  
end do  
end select  
call Coefficients(FlowType,Flowdir,Nx,Ny,Nz,Dx,Dy,Dz)  
call SOR(Neq,LocPar%ErrSOR,LocPar%Omega)  
if (FlowType<3) then  
call GradVol(FlowDir,KeffZ,Nx,Ny,Nz,Dx,Dy,Dz)  
else  
call GradSurf(FlowDir,KeffZ,Nx,Ny,Nz,Dx,Dy,Dz)  
end if  
deallocate(a,stat=err)  
deallocate(ita,stat=err)  
deallocate(lne,stat=err)  
deallocate(b,stat=err)  
deallocate(q,stat=err)  
deallocate(mat,stat=err)  
deallocate(mat1,stat=err)  
if (FlowType==3) then  
deallocate(xx,stat=err)  
deallocate(yy,stat=err)  
deallocate(zz,stat=err)  
end if  
99 continue  
end subroutine ComKeff

end module local

B.6 Module input.f90

module input  
! contains DPOR1D procedure for reading data file  
use globals  
use soilfunc  
imPLICIT none  
contains  
subroutine ReadData(ff,macro,block,soil1,soil2,par,icondf,icondb,&  
ubcond,ibcond,ptimes,problemname,problemtext,locpar,Keff2)  
imPLICIT none

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Appendix B. DPOR–1D source code

type (TSoilPar) :: soil1, soil2

type (TMacroDis) :: macro

type (TMicroDis) :: block

type (TLocPar) :: locpar

type (TInitial) :: icondf, icondb

type (TBoundary) :: ubcond, lbcond

type (TNumPar) :: par

type (TPrint) :: ptimes

real(8) ar, arx, ary, arz, as, av, ke, KeffZ

integer ff, i, j, k

character(*) problemname, problemtext

5 format(a64)

read (ff,*)
read (ff,*)
read (ff,*) ProblemName
read (ff,*)
read (ff,5) ProblemText
read (ff,*)
read (ff,*) Macro%FlowType, Macro%FlowDir, Macro%Len, Macro%Lp
read (ff,*)
read (ff,*) Block%PerX, Block%PerY, Block%PerZ, Block%GeomType

Macro%Dz = Macro%Len / (Macro%Lp - 1)
Block%PerVol = Block%PerX * Block%PerY * Block%PerZ
Block%IncVol = Block%PerVol
Block%IncSNR = 0.
Block%IncSVR = 0.

select case (Block%GeomType)

case (0) ! no blocks

read (ff,*)
read (ff,*)
read (ff,*) Block%IncVol = 0.
Block%IncSNR = 0.
Block%IncSVR = 0.

case (1) ! vertical layers
if (Macro%FlowType == 3) then
  print *, 'Wrong geometry for this type of flow'
  stop
end if
read (ff,*) Block%IncX
read (ff,*) Block%IncY
Block%IncZ = Block%IncX / (Block%IncY - 1)
Block%IncSNR = Block%IncZ 
Block%IncSVR = Block%IncZ
Block%IncVol = Block%IncZ * Block%IncY * Block%IncX
Block%IncSNR = 2. * Block%IncZ
Block%IncSVR = 2. * Block%IncZ

case (2) ! vertical column
if (Macro%FlowType == 3) then
  print *, 'Wrong geometry for this type of flow'
  stop
end if
read (ff,*) Block%IncX, Block%IncY
read (ff,*) Block%IncZ
Block%IncSNR = Block%IncZ
Block%IncSVR = Block%IncZ
Block%IncVol = Block%IncZ * Block%IncY * Block%IncX

case (3) ! horizontal cylinder
read (ff,*) Block%IncX
read (ff,*) Block%IncY
read (ff,*) Block%IncZ
Block%IncSNR = Block%IncZ
Block%IncSVR = Block%IncZ
Block%IncVol = Block%IncZ * Block%IncY * Block%IncX

Appendix B. DPOR–1D source code

case (4) ! horizontal parallelepiped
read (ff,*) Block%IncX, Block%IncY
read (ff,*) Block%IncX, Block%IncY
read (ff,*) Block%IncX, Block%IncY
Block%DX=0.5*Block%IncX / (Block%LX-1)
Block%DY=0.5*Block%IncY / (Block%LY-1)
Block%LP=Block%LX*Block%LY
Block%LZ=1
Block%IncVol=Block%IncX*Block%IncY*Block%IncZ
Block%IncSurf = 2.* (Block%IncX*Block%IncY*Block%IncZ)
Block%IncSVR = Block%IncSurf / Block%IncVol

case (5) ! spheres
read (ff,*) Block%IncX
read (ff,*) Block%IncX
read (ff,*) Block%IncX
Block%DX=Block%IncX / (Block%LX-1)
Block%LP=Block%LX
Block%LY=1
Block%LZ=1
Block%IncVol=4./3.*pi*Block%IncX**3.
Block%IncSurf=4*pi*Block%IncX**2.
Block%IncSVR=Block%IncSurf / Block%IncVol

case (6) ! parallelepipeds
read (ff,*) Block%IncX, Block%IncY, Block%IncZ
read (ff,*) Block%IncX, Block%IncY, Block%IncZ
read (ff,*) Block%IncX, Block%IncY, Block%IncZ
Block%DX=0.5*Block%IncX / (Block%LX-1)
Block%DY=0.5*Block%IncY / (Block%LY-1)
Block%DL=Block%LX*Block%LY*Block%LZ
Block%IncVol=Block%IncX*Block%IncY*Block%IncZ
Block%IncSurf = 2.*Block%IncX*Block%IncY*2.*Block%IncX*Block%IncY*2.*Block%IncZ
Block%IncSVR = Block%IncSurf / Block%IncVol

case (7) ! centered spheres
read (ff,*) Block%IncX
read (ff,*) Block%IncX
read (ff,*) Block%IncX
Block%DX=Block%IncX / (Block%LX-1)
Block%LP=Block%LX
Block%LY=1
Block%LZ=1
Block%IncVol=2.*4./3.*pi*Block%IncX**3.
Block%IncSurf=2.*4*pi*Block%IncX**2.
Block%IncSVR=Block%IncSurf / Block%IncVol

case (8) ! centered parallelepipeds
read (ff,*) Block%IncX, Block%IncY, Block%IncZ
read (ff,*) Block%IncX, Block%IncY, Block%IncZ
read (ff,*) Block%IncX, Block%IncY, Block%IncZ
Block%DX=0.5*Block%IncX / (Block%LX-1)
Block%DY=0.5*Block%IncY / (Block%LY-1)
Block%DL=Block%LX*Block%LY*Block%LZ
Block%IncVol=2.*Block%IncX*Block%IncY*Block%IncZ
Block%IncSurf = 2.*Block%IncX*Block%IncY*2.*Block%IncX*Block%IncY*2.*Block%IncZ*Block%IncY
Block%IncSVR = Block%IncSurf / Block%IncVol

end select

Soil1%Ke=1.
soil2%Ke=1.
soil1%ss=1.d-6
soil2%ss=1.d-6
soil1%Av=Block%Vol1
if (Macro%FlowType==1) then
soil2%Av=0.
else
soil2%Av=Block%Vol2
end if

Block%Vol2=Block%IncVol/Block%PerVol
if (Block%GeoType==2.) Block%Vol2=1.-Block%Vol2
Block%Vol1=1.-Block%Vol2

write (*,*)'Block shape not specified !'
stop
end if
read (ff,*) LocPar%Flag, LocPar%Nxs, LocPar%Nys, LocPar%ErrSOR, LocPar%Omega, KeffZ
read (ff,*)
read (ff,*) Soil1%fctype, Soil1%lp
read (ff,*)
select case (Soil1%fctype)
case (1)
do i=1,Soil1%lp
  read (ff,*) Soil1%ph(i), Soil1%pt(i), Soil1%pk(i)
end do

case (2)
read (ff,*) Soil1%tetas, Soil1%tetar, Soil1%alpha, Soil1%ks
  Soil1%lm=1.-1./Soil1%ks


case (3)
read (ff,*) Soil1%tetas, Soil1%tetar, Soil1%alpha, Soil1%ks, Soil1%eta
  Soil1%ha=1./Soil1%alpha


case (4)
read (ff,*) Soil1%tetas, Soil1%tetar, Soil1%alpha, Soil1%ks, Soil1%eta
  Soil1%lm=1.-2./Soil1%ks, Soil1%ha=1./Soil1%alpha


case (5)
read (ff,*) Soil1%tetas, Soil1%tetar, Soil1%alpha, Soil1%ks
  Soil1%lm=1.-1./Soil1%ks
  Soil1%lp=10
  Soil1%ph(1)=-150.
  Soil1%pk(1)=1.29d-6
  Soil1%ph(2)=-200.
  Soil1%pk(2)=2.13d-7
  Soil1%ph(3)=-300.
  Soil1%pk(3)=6.92d-9
  Soil1%ph(4)=4.84d-10
  Soil1%ph(5)=500.
  Soil1%ph(6)=5.40d-11
  Soil1%ph(7)=600.
  Soil1%ph(8)=9.32d-12
  Soil1%ph(9)=700.
  Soil1%ph(10)=7.22d-12
  Soil1%ph(11)=800.
  Soil1%ph(12)=5.82d-13
  Soil1%ph(13)=900.
  Soil1%ph(14)=6.87d-14

  case default
    write (*,*), 'Soil functions not specified !'
stop
end select
read (ff,*)
read (ff,*) Soil2%fctype, Soil2%lp
read (ff,*)
select case (Soil2%fctype)
case (1)
do i=1,Soil2%lp
  read (ff,*) Soil2%ph(i), Soil2%pt(i), Soil2%pk(i)
end do

case (2)
read (ff,*) Soil2%tetas, Soil2%tetar, Soil2%alpha, Soil2%ks
  Soil2%lm=1.-1./Soil2%ks


case (3)
read (ff,*) Soil2%tetas, Soil2%tetar, Soil2%alpha, Soil2%ks, Soil2%eta
  Soil2%ha=1./Soil2%alpha


case (4)
read (ff,*) Soil2%tetas, Soil2%tetar, Soil2%alpha, Soil2%ks, Soil2%eta
  Soil2%lm=1.-2./Soil2%ks, Soil2%ha=1./Soil2%alpha

  case default
    write (*,*) 'Soil functions not specified !'
stop
end select
read (ff,*)
read (ff,*) icondf%fctype, icondf%upvalue
read (ff,*)
read (ff,*) icondb%fctype, icondb%upvalue
read (ff,*)
read (ff,*) ubcond%fctype, ubcond%lp
read (ff,*)
do i=1, ubcond%lp
  read (ff,*) ubcond%times(i), ubcond%values(i)
end do
read (ff,*)
do i=1, 1bcond%lp

read (ff,*) lbcond%times(i), lbcond%values(i)
end do

read (ff,*) par%Beta, par%SourceType
read (ff,*) par%DtInit, par%DtMin, par%DtMax
read (ff,*) par%NItMax, par%ErrOpt1, par%ErrOpt2, par%Mul1, par%Mul2
read (ff,*) par%AbsTol, par%RelTol
read (ff,*) ptimes%lp
read (ff,*) (ptimes%times(i), i=1, ptimes%lp)
do i=1, ptimes%lp
   ptimes%times(i)=ptimes%times(i)
end do
read (ff,*) Macro%Nobs
if (Macro%nobs>0) then
   read (ff,*) (ZCor(i),i=1,Macro%NObs)
end if
do i=1, Macro%NObs
   if (ZCor(i)>Macro%Len) then
      print *, 'Observation nodes outside solution domain'
      stop
   end if
   Macro%ObsInd(i)=nint(ZCor(i)/Macro%Dz)+1
end do
end subroutine ReadData

!----------------------------------------------------------------
end module input

B.7 Module output.f90

module output
! contains subroutines controlling
! the output files
use globals
use soilfunc
contains
!************************************************************************
subroutine DataSum(ff,dmain,dblock,soil1,soil2,icondf,icondb,ubcond,&
lbcond,par,ptimes)
implicit none
type (TSoilPar):: soil1,soil2
type (TMacroDis):: dmain
type (TMicroDis):: dblock
type (TInitial):: icondf,icondb
type (TBoundary):: ubcond, lbcond
type (TRunPar):: par
type (TPrint):: ptimes
type (TMassBal):: bal
type (TRunTime):: time
integer ff,i

write (ff,*) 'DOMAIN GEOMETRY'
write (ff,31) 'Macroscopic domain length [L]',dmain%Len
write (ff,31) 'Space step DZ [L]',dmain%Dz
write (ff,33) 'X,Y,Z period dim. [L]',dblock%PerX,dblock%PerY,dblock%PerZ
write (ff,31) 'Period volume [L3]',dblock%PerVol
write (ff,*) 'Period volume [L3]',dblock%PerVol
write (ff,*)
write (ff,31) 'INCLUSION GEOMETRY'
select case (dblock%GeomType)
case (0)
   write (ff,*) 'No inclusions'
case (1)
write (ff,*) 'Vertical layers'
write (ff,31) 'Layer width [L], dblock%IncX
write (ff,31) 'DX [L], dblock%Dx

case (2)
write (ff,*) 'Vertical column (rectangular)'
write (ff,33) 'X,Y inner dimensions [L], dblock%IncX, dblock%IncY
write (ff,33) 'DX, DY [L], dblock%Dx, dblock%Dy

case (3)
write (ff,*) 'Inclusion shape : cylinder'
write (ff,31) 'Radius [L], dblock%IncX
write (ff,31) 'DR [L], dblock%Dx

case (4)
write (ff,*) 'Horizontal solid column (rectangular)'
write (ff,33) 'X,Y outer dimensions [L], dblock%IncX, dblock%IncY
write (ff,33) 'DX, DY [L], dblock%Dx, dblock%Dy

case (5)
write (ff,*) 'Inclusion shape : spheres (simple arrangement)
write (ff,31) 'Radius [L], dblock%IncX
write (ff,31) 'DR [L], dblock%Dx

case (6)
write (ff,*) 'Inclusion shape : parallelepiped (simple arrangement)'
write (ff,33) 'X,Y,Z block dim. [L], dblock%IncX, dblock%IncY, dblock%IncZ
write (ff,33) 'DX, DY, DZ [L], dblock%Dx, dblock%Dy, dblock%Dz

end select
write (ff,31) 'Block volume [L3], dblock%IncVol
write (ff,31) 'Specific surface [-/L], dblock%IncSVR
write (ff,*)
write (ff,31) 'Region 1 volume ratio [-], dblock%Vol1
write (ff,31) 'Region 2 volume ratio [-], dblock%Vol2
write (ff,*)
select case (soil1%ftype)

case (1)
write (ff,*) 'REGION 1: Tabularized hydraulic functions'
write (ff,36) 'H [L], TH [-], K [L/T],
do i=1,soil1%lp
write (ff,36) soil1%ph(i), soil1%pt(i), soil1%pk(i)
end do

case (2)
write (ff,*) 'REGION 1: TH(H): Van Genuchten - Mualem model, K(H): Mualem model'
write (ff,31) 'KS [L/T], soil1%ks
write (ff,31) 'ThetaS [-], soil1%thetaS
write (ff,31) 'ThetaR [-], soil1%thetaR
write (ff,31) 'Alpha [-/L], soil1%alpha


case (3)
write (ff,*) 'REGION 1: TH(H): Brooks - Corey model, K(H): Brooks - Corey model'
write (ff,31) 'KS [L/T], soil1%ks
write (ff,31) 'ThetaS [-], soil1%thetaS
write (ff,31) 'ThetaR [-], soil1%thetaR
write (ff,31) 'Alpha [-/L], soil1%alpha
write (ff,31) 'N [-], soil1%n
write (ff,31) 'Eta [-], soil1%eta


case (4)
write (ff,*) 'REGION 1: TH(H): Van Genuchten - Burdine model, K(H): Brooks - Corey model'
write (ff,31) 'KS [L/T], soil1%ks
write (ff,31) 'ThetaS [-], soil1%thetaS
write (ff,31) 'ThetaR [-], soil1%thetaR
write (ff,31) 'Alpha [-/L], soil1%alpha
write (ff,31) 'N [-], soil1%n
write (ff,31) 'Eta [-], soil1%eta

end select
Appendix B. DPOR–1D source code

end select
write (ff,*)
select case (soil2%ftype)
case (1)
write (ff,*') 'REGION 2: Tabularized hydraulic functions'
write (ff,35) 'h [L]', 'th [-]', 'k [L/T]' 
do i=1,soil2%lp
write (ff,36) soil2%ph(i),soil2%pt(i),soil2%pk(i)
end do
case (2)
write (ff,*') 'REGION 2: TH(H): Van Genuchten – Mualem model, K(H): Mualem model'
write (ff,31) 'KS [L/T]',soil2%ks
write (ff,31) 'ThetaS [-]',soil2%tetas
write (ff,31) 'ThetaR [-]',soil2%tetar
write (ff,31) 'Alpha [-/L]',soil2%alfa
write (ff,31) 'N [-]',soil2%n
case (3)
write (ff,*') 'REGION 2: TH(H): Brooks – Corey model, K(H): Brooks – Corey model'
write (ff,31) 'KS [L/T]',soil2%ks
write (ff,31) 'ThetaS [-]',soil2%tetas
write (ff,31) 'ThetaR [-]',soil2%tetar
write (ff,31) 'Alpha [-/L]',soil2%alfa
write (ff,31) 'N [-]',soil2%n
write (ff,31) 'Eta [-]',soil2%eta
case (4)
write (ff,*') 'REGION 2: TH(H): Van Genuchten – Burdine model, K(H): Brooks – Corey model'
write (ff,31) 'KS [L/T]',soil2%ks
write (ff,31) 'ThetaS [-]',soil2%tetas
write (ff,31) 'ThetaR [-]',soil2%tetar
write (ff,31) 'Alpha [-/L]',soil2%alfa
write (ff,31) 'N [-]',soil2%n
write (ff,31) 'Eta [-]',soil2%eta
end select
write (ff,*)
select case (dmain%FlowType)
case (3)
write (ff,*') 'Region 1 not connected: Equilibrium flow'
write (ff,31) 'KS effective [-]',soil2%ke*soil2%ks
write (ff,31) 'KS EFF / KS2 [-]',soil2%ke
case (2)
write (ff,*') 'Region 1 connected: Equilibrium flow'
write (ff,31) 'KS effective [-]',soil1%ke*soil1%ks
write (ff,31) 'KS EFF / KS2 [-]',soil1%ke
case (1)
write (ff,*') 'Region 1 connected: Non-equilibrium flow'
write (ff,31) 'KS effective [-]',soil1%ke*soil1%ks
write (ff,31) 'KS EFF / KS2 [-]',soil1%ke
case (0)
write (ff,*') 'Homogeneous medium (region 1): Equilibrium flow'
end select
write (ff,*)
if (icondf%ctype==1) then
write(ff,*') 'INITIAL CONDITION IN REGION 1: Uniform pressure distribution'
write(ff,31) 'Top value [L]',icondf%upvalue
write(ff,31) 'Bottom value [L]',icondf%upvalue+icondf%dz
else
write(ff,*') 'INITIAL CONDITION IN REGION 1: Hydrostatic pressure distribution'
write(ff,31) 'Top value [L]',icondf%upvalue+(dmain%lp-1)*dmain%dz
end if
write (ff,*)
if (icondb%ctype==1) then
write(ff,*') 'INITIAL CONDITION IN REGION 2: Uniform pressure distribution'
write(ff,31) 'Top value [L]',icondb%upvalue
write(ff,31) 'Bottom value [L]',icondb%upvalue+icondb%dz
else
write(ff,*') 'INITIAL CONDITION IN REGION 2: Hydrostatic pressure distribution'
write(ff,31) 'Top value [L]',icondb%upvalue+(dmain%lp-1)*dmain%dz
end if
write (ff,*)
if (ubcond%ctype==1) then
write(ff,*') 'TOP BOUNDARY CONDITION: Pressure'
write (ff,32) 't [T]', 'h [L]' 
do i=1,ubcond%lp
write (ff,34) ubcond%times(i),ubcond%values(i)
end do
Appendix B. DPOR–1D source code

else if (ubcond%ctype==2) then
  write(ff,*), 'TOP BOUNDARY CONDITION: Flux'
  write (ff,32) 't [T]', 'qt [L/T]'
  do i=1,ubcond%lp
    write (ff,34) ubcond%times(i),ubcond%values(i)
  end do
end if
write (ff,*)
if (lbcond%ctype==1) then
  write(ff,*), 'BOTTOM BOUNDARY CONDITION: Pressure'
  write (ff,32) 't [T]', 'hb [L]'  
  do i=1,lbcond%lp
    write (ff,34) lbcond%times(i),lbcond%values(i)
  end do
else if (lbcond%ctype==2) then
  write(ff,*), 'BOTTOM BOUNDARY CONDITION: Flux'
  write (ff,32) 't [T]', 'qb [L/T]'  
  do i=1,lbcond%lp
    write (ff,34) lbcond%times(i),lbcond%values(i)
  end do
else if (lbcond%ctype==3) then
  write (ff,*), 'BOTTOM BOUNDARY CONDITION: Free drainage'
end if
write (ff,*)
write (ff,*) 'NUMERICAL PARAMETERS:'
write (ff,31) 'Weighting parameter [-]: ',par%beta
write (ff,31) 'Initial time step [T]: ',par%DtInit
write (ff,31) 'Minimum allowable time step [T]: ',par%DtMin
write (ff,31) 'Maximum allowable time step [T]: ',par%DtMax
write (ff,31) 'Absolute tolerance [L]: ',par%AbsTol
write (ff,31) 'Relative tolerance [-]: ',par%RelTol
write (ff,31) 'Source term calculation: ',par%SourceType
write (ff,*) 'Print times [T]'
do i=1,ptimes%lp
  write (ff,37) ptimes%times(i)
end do
write (ff,*)
write (ff,*) 'Observation points [L]'
do i=1,dmain%NObs
  write (ff,37) (dmain%ObsInd(i)-1)*dmain%dz
end do
Appendix B. DPOR–1D source code

subroutine WriteLocalProf(ff,maxeq,maxbl,hblock,dmain,dblock,t)
 implicit none
 integer maxeq,maxbl
 type(TMacroDis):: dmain
 type(TMicroDis):: dblock
 real(8) hblock(maxeq,maxbl),t
 integer ff,i,j,k,kk,np
 write (ff,*)
 write (ff,50)
 write (ff,5) 'T [T] ',t
 write (ff,50)
 write (ff,7) 'Y1 [L]','Y2 [L]','Y3 [L]','H2 [L]',('H2 [L]',kk=1,dmain%Nobs)
 write (ff,50)
 do i=1,dblock%lx
  do j=1,dblock%ly
   do k=1,dblock%lz
    np=i+(j-1)*dblock%lx+(k-1)*dblock%lx*dblock%ly
    write (ff,10) (i-1)*dblock%dx,(j-1)*dblock%dy,(j-1)*dblock%dz, (hblock(dmain%ObsInd(kk),np),kk=1,dmain%Nobs)
   end do
  end do
 end do
 write (ff,*)
 write (ff,60)
 5 format (a12,es12.3)
 7 format (13a12)
 10 format (13es12.3)
 50 format (76('-'))
 60 format (76('*'))
 end subroutine WriteLocalProf

subroutine WriteLevel(ff1,ff2,par,bal)
 implicit none
 type(TNumPar)::par
 type(TMassBal)::bal
 integer ff1,ff2
 write (ff1,25) par%ndt,par%t,par%lastdt,par%niter,par%titer
 write (ff2,35) par%t,bal%tqin,bal%tqout,bal%tsource,bal%wfin,bal%wbfin,&
 bal%balance,bal%relbalance
 25 format (i12,2es12.3)
 35 format (8es12.3)
 end subroutine WriteLevel

subroutine WriteObs(i,ff,maxeq,h,tet,kk,qq,sq,&
 hmean,tetmean,dmain,t)
 implicit none
 integer i,ff,np,maxeq
 real(8) h(maxeq),tet(maxeq),qq(maxeq),sq(maxeq),kk(maxeq),&
 hmean(maxeq),htetmean(maxeq),t
 type(TMacroDis):: dmain
 np=dmain%ObsInd(i)
 write (ff,10) t,h(np),tet(np),kk(np),qq(np),-sq(np),hmean(np),tetmean(np) !,veloc(np),diff(np)
 10 format(10es12.3)
 end subroutine WriteObs

subroutine WriteRunInfo(ff,par,bal,time)
 implicit none
 type(TRunTime):: time
 type(TNumPar):: par
 type(TMassBal):: bal
 integer ff
 time%rtime=time%fday*24*3600.+time%fhr*3600+time%fmin*60.+time%fsec&
 -time%iday*24*3600.-time%ihr*3600-time%imin*60.-time%isec
 write (ff,*)
 end subroutine WriteRunInfo
write (ff,30) 'Start date and time',&
  time%iyear,time%imonth,time%iday,time%ihr,time%imin,time%isec
write (ff,30) 'End date and time',&
  time%fyear,time%fmonth,time%fday,time%fhr,time%fmin,time%fsec
write (ff,20) 'Total number of iterations [-]',par%ntiter
write (ff,20) 'Number of time steps [-]',par%ndt
write (ff,15) 'Smallest time step [T]',par%mindt
write (ff,15) 'Largest time step [T]',par%maxdt
write (ff,15) 'Cumulative top flux [L]',bal%tqin
write (ff,15) 'Cumulative bottom flux [L]',bal%tqout
write (ff,15) 'Initial water content (region 1) [L]',bal%winit
write (ff,15) 'Initial water content (region 2) [L]',bal%winit2
write (ff,15) 'Final water content (region 1) [L]',bal%wfin
write (ff,15) 'Final water content (region 2) [L]',bal%wfin2
write (ff,15) 'Absolute mass balance error [L]',bal%relbalance
write (ff,15) 'Relative mass balance error [%]',bal%relbalance
write (ff,15) 'Run time [s]',time%rtime
15 format (a37,es12.3)
20 format (a37,i8)
30 format (a37,i7,'/',i2,'/',i2,' ',i2,':',i2,':',i2)
end subroutine WriteRunInfo

!****************************************************************
subroutine Heading(ff,problemname,problemtext)
implicit none
integer ff,i
character(*) problemname, problemtext
write(ff,*) 'DPOR_1D output file'
write(ff,60)
write(ff,*) problemname
write(ff,60)
write(ff,*) problemtext
write(ff,60)
write(ff,5)
write(ff,*)
write(ff,5) 'Observation node: ',i
write(ff,*)
write(ff,10) 'Z [cm]',dmain%dz*(dmain%ObsInd(i)-1)
5 format(a20,i8)
10 format(a8,f12.3)
20 format(8a12)
50 format(76('-'))
60 format(76('*'))
end subroutine HeadingObs

!******************************************************************************
subroutine HeadingObs(i,ff,problemname,problemtext,dmain)
implicit none
integer ff,i,j
character(*) problemname, problemtext
type(TMacroDis):: dmain
write(ff,'*') 'DPOR_1D output file'
write(ff,60)
write(ff,*) problemname
write(ff,60)
write(ff,*) problemtext
write(ff,60)
write(ff,5)
write(ff,*)
write(ff,5) 'Observation node: ',i
write(ff,*)
write(ff,10) 'Z [cm]',dmain%dz*(dmain%ObsInd(i)-1)
5 format(a37,es12.3)
10 format(a8,f12.3)
20 format(8a12)
50 format(76('-'))
60 format(76('*'))
end subroutine HeadingObs
module MacSolv
!
contains subroutines for numerical solution
' of macroscopic equation
!
use globals
use soilfunc
use auxsub
use micsolv
!
contains
!

subroutine MacNewton(Maxeq,Maxbl,HOld,HTemp,HNew,ThOld,ThNew,KOld,KNew,ExOld,ExNew,&
HBlockOld,HBlockNew,ThBlockOld,ThBlockNew,KBlockOld,KBlockNew,&
ThAverOld,ThAverNew,HAver,par,dmain,dblock,soil1,soil2,ubcond,lbcond)
!
integer Maxeq,Maxbl
!
type (TSoilPar):: soil1,soil2,soilm
!
type (TMacroDis):: dmain
!
type (TMicroDis):: dblock
!
type (TBoundary):: ubcond, lbcond
!
type (TNumPar):: par
!
real(8) hOld(maxeq),ThOld(maxeq),ThNew(maxeq),hTemp(maxeq),hNew(maxeq),&
KOld(maxeq),KNew(maxeq),ExOld(maxeq),ExNew(maxeq),DExNew(maxeq),&
HBlockOld(maxeq,maxbl),HBlockNew(maxeq,maxbl),&
ThBlockOld(maxeq,maxbl),ThBlockNew(maxeq,maxbl),&
KBlockOld(maxeq,maxbl),KBlockNew(maxeq,maxbl),&
ThAverOld(maxeq),ThAverNew(maxeq),HAver(maxeq),&
HFirst(maxeq),HFirst(maxeq),zz(maxeq),&
wo(maxeq),w1(maxeq),w2(maxeq),a(maxeq),b(maxeq),c(maxeq),dh(maxeq),&
t,dt,dz,beta,k1,k2,Eps,k1n,k2n,k3n,k4n,cin,&
cf,cf1,dq1,dq2,dq3,dq4,hbb,hbt,qb0,qb,q0,qt,delta
!
integer i,j,lp,ii
!
logical endcalc
!
lp=dmain%lp
!
t=par%t
!
dz=dmain%dz
!
beta=par%beta
!
par%niter=0
!
cin=dmain%FlowDir
!
Eps=1.d-4
!
if (ubcond%ctype==1) then
    hbt=Bvalue(t+dt,ubcond)
else if (ubcond%ctype==2) then
    qt0=Bvalue(t,ubcond)
    qt=Bvalue(t+dt,ubcond)
end if
!
if (lbcond%ctype==1) then
    hbb=Bvalue(t+dt,ubcond)
else if (ubcond%ctype==2) then
    qb0=Bvalue(t,ubcond)
    qb=Bvalue(t+dt,ubcond)
end if
!
end if
!
end subroutine MacNewton
!
Appendix B. DPOR–1D source code

! else
! condition=2
! qbo=0.0d0
! qbo=0.0d0
! end if
!

if (dmain%FlowType==1).and.(par%SourceType>0) then
    call SourceTerm(Maxeq,Maxbl,HTemp,HBlockOld,HBlockNew,ThBlockOld,ThBlockNew,&
    Soil1,Soil2,dmain,dblock)
else
    ExNew=0.
    DExNew=0.
end if

w0=0.
k1=0.5*(KOld(1)+KOld(2))
do i=2,lp-1
    k2=0.5*(KOld(i)+KOld(i+1))
    w0(i)=cf*(k2*(HOld(i+1)-HOld(i))-k1*(HOld(i)-HOld(i-1))-cin*(k2-k1)*dz)+ThOld(i)&
    +(1.-beta)*ExOld(i)*dt
k1=k2
end do

call ComWaterEff(lp,HTemp,ThNew,soil1,soil2)
call ComK(lp,HTemp,KNew,soilm)
HFirst=HTemp
ExFirst=ExNew

do
    a=0
    b=0
    c=0
    w1=0
    k1=0.5*(KNew(1)+KNew(2))
    k1n=0.5*(Fkh(HTemp(1)+Eps,soilm)+KNew(2))
    dq1=cf1*((k1n*(HTemp(2)-HTemp(1)-Eps)-cin*k1n*dz)-(k1*(HTemp(2)-HTemp(1))-cin*k1*dz))/Eps
    k3n=0.5*(Fkh(HTemp(1)+Eps,soilm)+KNew(1))
    dq3=cf1*((k3n*(HTemp(2)-HTemp(1))-cin*k3n*dz)-(k1*(HTemp(2)-HTemp(1))-cin*k1*dz))/Eps
    k4n=0.5*(KNew(1)+Fkh(HTemp(2)+Eps,soilm))
    dq4=cf1*((k4n*(HTemp(2)+Eps-HTemp(1))-cin*k4n*dz)-(k2*(HTemp(2)-HTemp(1))-cin*k2*dz))/Eps
    c(i)=(soil1%av*FTheta(HTemp(i)+Eps,soilm)+soil2%av*FTheta(HTemp(i)+Eps,soilm)-ThNew(i))/Eps
    c(i)=0.5*soil1%av*FCap(HTemp(i),soilm)+0.5*soil2%av*FCap(HTemp(i),soilm)
    c(i)=c(i)-dq2-dq3-beta*DExNew(i)*dt
    a(i)=dq1
    b(i)=-dq4
    w2(i)=w1(i)+w0(i)+beta*ExNew(i)*dt
    k1=k2
    dq1=dq3
    dq2=dq4
end do

! upper boundary condition
if (ubcond%ctype==1) then
    ! specified head
    a(1)=0.
    b(1)=0.
    c(1)=1.
    w2(1)=hbt-HTemp(1)
else
    ! specified flux
    k2=0.5*(KOld(1)+KOld(2))
    w0(1)=cf*(k2*(HOld(2)-HOld(1))-cin*k2*dz+qto*dz)+0.5*ThOld(1)
    k2=0.5*(KNew(1)+KNew(2))
    w1(1)=cf*(k2*(HTemp(2)-HTemp(1))-cin*k2*dz+qto*dz)-0.5*ThNew(1)
    k3=0.5*(Fkh(HTemp(1)+Eps,soilm)+KNew(1))
    dq3=cf1*((k3n*(HTemp(2)-HTemp(1))-cin*k3n*dz)-(k2*(HTemp(2)-HTemp(1))-cin*k2*dz))/Eps
    k4=0.5*(KNew(1)+Fkh(HTemp(2)+Eps,soilm))
    dq4=cf1*((k4n*(HTemp(2)+Eps-HTemp(1))-cin*k4n*dz)-(k2*(HTemp(2)-HTemp(1))-cin*k2*dz))/Eps
    c(i)=(soil1%av*FTheta(HTemp(i)+Eps,soilm)+soil2%av*FTheta(HTemp(i)+Eps,soilm)-ThNew(i))/Eps
    c(i)=c(i)+a(i)*dt
    b(i)=-dq4
    w2(1)=w1(1)+w0(1)+dt*(beta*ExNew(1)+(1.-beta)*ExOld(1))
end if

! lower boundary condition
select case (lbcond%ctype)
case(1)
    ! specified head
    a(lp)=0.
    b(lp)=0.
    c(lp)=1.
    w2(lp)=hbb-HTemp(1)
endif
case(2)
! specified flux
k1=0.5*(KOld(lp-1)+KOld(lp))
w0(lp)=cf*(-k1*(HOld(lp)-HOld(lp-1))+cin*k1*dz)+0.5*ThOld(lp)
k1=0.5*(KNew(lp-1)+KNew(lp))
w1(lp)=cf*(-k1*(HTemp(lp-1)-HTemp(lp-1))+cin*k1*dz-qb0*dz)+0.5*ThOld(lp)
k3=0.5*(FKh(HTemp(lp-1)+Eps,soilm)+KNew(lp))
dq3=cf1*((k3*(HTemp(lp)-HTemp(lp-1))-cin*k3*dz)/(1.*(HTemp(lp)-HTemp(lp-1))-cin*k3*dz))/Eps
k1=0.5*(KNew(lp-1)+Fkh(HTemp(lp)+Eps,soilm))
w1(lp)=cf1*(-k1*(HTemp(lp)-HTemp(lp-1))+cin*k1*dz-qb*dz)-0.5*ThNew(lp)
k3n=0.5*(FKh(HTemp(lp-1)+Eps,soilm)+KNew(lp))
dq3=cf1*((k3n*(HTemp(lp)-HTemp(lp-1))-cin*k3n*dz)/(1.*(HTemp(lp)-HTemp(lp-1))-cin*k3n*dz))/Eps
! c(lp)=(soil1%av*FTheta(HTemp(lp-1)+Eps,soil1)+soil2%av*FTheta(HTemp(lp-1)+Eps,soil2)-ThNew(lp))/Eps
! c(lp)=soil1%av*FCap(HTemp(lp),soil1)+soil2%av*FCap(HTemp(lp),soil2)
c(lp)=c(lp)+dq3-beta*DExNew(lp)*dt
a(lp)=dq3
b(lp)=0.
w2(lp)=w1(lp)+w0(lp)+dt*(beta*ExNew(lp)+(1.-beta)*ExOld(lp))
case(3)
! free drainage (zero gradient)
k1=0.5*(KOld(lp-1)+KOld(lp))
k2=KOld(lp)
w1(lp)=cf*(-k1*(HOld(lp)-HOld(lp-1))+cin*k1*dz-cin*k2*dz)+ThOld(lp)
k1=0.5*(KNew(lp-1)+KNew(lp))
k2=KNew(lp)
! c(lp)=(soil1%av*FTheta(HTemp(lp-1)+Eps,soil1)+soil2%av*FTheta(HTemp(lp-1)+Eps,soil2)-ThNew(lp))/Eps
! c(lp)=soil1%av*FCap(HTemp(lp),soil1)+soil2%av*FCap(HTemp(lp),soil2)
c(lp)=c(lp)+k1*cf1 !-beta*DExNew(lp)*dt
a(lp)=-k1*cf1
b(lp)=0.
w2(lp)=w1(lp)+cf1*(-k1*(HTemp(lp)-HTemp(lp-1))+cin*k1*dz-cin*k2*dz)-ThNew(lp) !+dt*(beta*ExNew(lp)+(1.-beta)*ExOld(lp))
end select
!---------------------------------------------------------------------------------
call Thomas(lp,a,b,c,w2,dh)
HNew=HTemp+dh
if ((dmain%FlowType==1).and.(par%SourceType>0)) then
if (par%SourceType==1) then
ExNew=ExFirst+DExNew*(HNew-HFirst)
else
call SourceTerm(Maxeq,Maxbl,HNew,HBlockOld,HBlockNew,ThBlockOld,ThBlockNew,&
KBlockOld,KBlockNew,ThAverOld,ThAverNew,HAver,ExNew,DExNew,&
soil1,par,dmain,dblock)
end if
end if
par%niter=par%niter+1
call ComWaterEff(lp,HNew,ThNew,soil1,soil2)
call ComK(lp,HNew,KNew,soilm)
!-----------------------------------------------------------------------------
!checking for termination of iterations
call termin(lp,HTemp,HNew,0.5*par%AbsTol,0.5*par%RelTol,endcalc)
if (endcalc.or.(par%niter>=par%NItMax)) exit
HTemp=HNew
end do ! end of main loop
par%niter=par%niter+1
d end subroutine MacNewton

!**************************************************************************
subroutine SourceTerm(Maxeq,Maxbl,HNew,HBlockOld,HBlockNew,ThBlockOld,ThBlockNew,&
KBlockOld,KBlockNew,ThAverOld,ThAverNew,HAver,ExNew,DExNew,&
soil1,par,dmain,dblock)
! computes the exchange of water between regions
! solves microscopic flow equations in periods
implicit none
integer Maxeq,Maxbl
type (TSoilPar):: soil
type (TMacroDis):: dmain,dcol
!**************************************************************************
real(8) HBlocOld(maxeq,maxb1),HBlocNew(maxeq,maxb1),ThBlockOld(maxeq,maxb1),&
ThBlockNew(maxeq,maxb1),KBlockOld(maxeq,maxb1),KBlockNew(maxeq,maxb1),&
ExNew(maxeq),DExNew(maxeq),HNew(maxeq),ThAverOld(maxeq),ThAverNew(maxeq),&
HAver(maxeq), HTemp0(MaxBl), HTemp1(MaxBl),&
KTemp0(MaxBl),KTemp1(MaxBl), TTemp0(MaxBl), TTemp1(MaxBl),rr(MaxBl),&
Eps,dz,bhound,bbound1,thetanev,thetaNew1,Expom,wf,wf1,ssq,cf
integer i,j,k,lp,lk,nbl,HBound(MaxBl)
!-----------------------------------------------------------------------------
lp@dmain%lp
lk@dblock%lp
dz=dmain%dz
Eps=1.0d-1
cf=dblock%vol2
if (dblock%geomtype==6) then
!boundary nodes
NNB=dblock%lx*dblock%ly*dblock%lx*dblock%ly*dblock%lx*dblock%lx
k=1
do i=1,dblock%lx
   do j=1,dblock%ly
      NBound(k)=i+(j-1)*dblock%lx
      k=k+1
   end do
end do
do i=1,dblock%lx
   do j=1,dblock%ly
      NBound(k)=i+(j-1)*dblock%lx*dblock%ly
      k=k+1
   end do
end do
do i=1,dblock%lx*dblock%ly
   ! boundary nodes are added to domain nodes
   ! choose all nodes in the boundary
end do
end if

do i=1,DBlock%Lp
   Rr(i)=(i-1)*DBlock%Dx
end do

do i=1,lp
   do j=1,lk
      HTemp0(j)=HBlockOld(i,j)
      HTemp1(j)=HBlockOld(i,j)
      KTemp0(j)=KBlockOld(i,j)
      KTemp1(j)=KBlockOld(i,j)
      TTemp0(j)=ThBlockOld(i,j)
      TTemp1(j)=ThBlockOld(i,j)
   end do
   HBound=HNew(i)
   HBound1=HBound+Eps
   select case (dblock%GeomType)
   !--------------------------------------------------------------------------------
   case (1) ! parallel fractures
   dcol%dz=dblock%dx
   dcol%lp=dblock%lp
   call Newton1d(Maxbl,HTemp0,HTemp1,TTemp0,TTemp1,KTemp0,KTemp1,&
   par,dcol,soil,hbound1,1,ThetaNew1)
   call Newton1d(Maxbl,HTemp0,HTemp1,TTemp0,TTemp1,KTemp0,KTemp1,&
   par,dcol,soil,hbound,1,ThetaNew)
   !--------------------------------------------------------------------------------
   case (2) ! vertical columns
   call Solve2DHollow(Maxbl,HTemp0,HTemp1,TTemp0,TTemp1,KTemp0,KTemp1,&
   dblock,soil,par,HBound1,ThetaNew1)
   call Solve2DHollow(Maxbl,HTemp0,HTemp1,TTemp0,TTemp1,KTemp0,KTemp1,&
   dblock,soil,par,HBound,ThetaNew)
   !--------------------------------------------------------------------------------
   case (3) ! horizontal cylinders
   call SolveCylinder(Maxbl,HTemp0,HTemp1,TTemp0,TTemp1,KTemp0,KTemp1,&
   par,dblock,soil,hBound1,ThetaNew1,rr)
   call SolveCylinder(Maxbl,HTemp0,HTemp1,TTemp0,TTemp1,KTemp0,KTemp1,&
   par,dblock,soil,hBound,ThetaNew,rr)
   !--------------------------------------------------------------------------------
   case (4) ! horizontal columns
   call Solve2DSolid(Maxbl,HTemp0,HTemp1,TTemp0,TTemp1,KTemp0,KTemp1,&
   dblock,soil,par,HBound1,ThetaNew1)
   call Solve2DSolid(Maxbl,HTemp0,HTemp1,TTemp0,TTemp1,KTemp0,KTemp1,&
   dblock,soil,par,HBound,ThetaNew)
   !--------------------------------------------------------------------------------
   case (5,7) ! spheres
   call SolveSphere(Maxbl,HTemp0,HTemp1,TTemp0,TTemp1,KTemp0,KTemp1,&
Appendix B. DPOR–1D source code

```fortran
par, dblock, soil, hBound1, ThetaNew1, rr)
call SolveSphere(maxbl, HTemp0, HTemp1, TTemp0, TTemp1, KTemp0, KTemp1, &
par, dblock, soil, hBound, ThetaNew, rr)
!
print *, i,
!--------------------------------------------------------------------------------
! case (6, 8) ! parallelepipeds

call Solve3d(Maxbl, HTemp0, HTemp1, TTemp0, TTemp1, KTemp0, KTemp1, &
dblock, soil, par, hbound1, ThetaNew1, NNB, hBound)
call Solve3d(Maxbl, HTemp0, HTemp1, TTemp0, TTemp1, KTemp0, KTemp1, &
dblock, soil, par, hbound, ThetaNew, NNB, hBound)
end select

ExNew(i) = -(dblock%Vol2*ThetaNew-ThAverOld(i))/par%dt
ssq1 = -(dblock%Vol2*ThetaNew1-ThAverOld(i))/par%dt
DExNew(i) = (ssq1-ExNew(i))/Eps
ThAverNew(i) = dblock%Vol2*ThetaNew
HAver(i) = FInvTheta(ThetaNew, soil)
do j=1, lk
HBlockNew(i,j)=HTemp1(j)
ThBlockNew(i,j)=TTemp1(j)
KBlockNew(i,j)=KTemp1(j)
end do
end do
!print *,maxval(ExNew)
end subroutine SourceTerm

!************************************************************************
!**************************************************************************************
end module macsolv

B.9 Module micsolv.f90

module MicSolv
!
! subroutines for the solution of local problem
! 1D - parallel fractures
! 2D - rectangular geometry
! 3D - hexahedral geometry
! circle, sphere
!
use Globals
use SoilFunc
use AuxSub
contains

!******************************************************************************
subroutine Newton1D(Maxdir, HOld, HNew, ThOld, ThNew, KOld, KNew, par, dmain, soil1, HBound, NBPoints, WCNew)
! solution of 1D microscopic flow equation
! no gravity, simple boundary conditions

implicit none
!
!!-------------------------------------------------------------------------------
integer Maxdir
!
type (TSoilPar):: soil1
!
type (TMacroDis):: dmain
!
type (TNumPar):: par
!
real(8) HOld(maxdir), HTemp(maxdir), HNew(maxdir), ThOld(maxdir), ThNew(maxdir), &
KOld(maxdir), KNew(maxdir), TTemp(maxdir), KTemp(maxdir), &
w0(maxdir), w1(maxdir), w2(maxdir), a(maxdir), b(maxdir), c(maxdir), d(maxdir), &
dz, dt, dz, beta, k1, k2, Eps, cf, cf1, dq1, dq2, dq3, dq4, hBound, k1n, k2n, k3n, k4n, WCNew
!
integer i, j, n, iter, lp, NBPoints, n11
!
logical endcalc
!
!-------------------------------------------------------------------------------
!
integer Maxdir
!
type (TSoilPar):: soil1
!
type (TMacroDis):: dmain
!
type (TNumPar):: par
!
real(8) HOld(maxdir), HTemp(maxdir), HNew(maxdir), ThOld(maxdir), ThNew(maxdir), &
KOld(maxdir), KNew(maxdir), TTemp(maxdir), KTemp(maxdir), &
dz, dt, dz, beta, k1, k2, Eps, cf, cf1, dq1, dq2, dq3, dq4, hBound, k1n, k2n, k3n, k4n, WCNew
!
integer i, j, n, iter, lp, NBPoints, n11
!
logical endcalc
!
lp=dmain%lp
dt=par%dt
dz=dmain%dz
beta=par%beta
Eps=1.d-3
n1=0
!
!
!
Eps=1.d-3
n1=0
!
!

! computing constant part of RHS vector
w0=0.
```

```
Appendix B. DPOR–1D source code

\[ k_1 = 0.5 \times (K_{Old}(1) + K_{Old}(2)) \]
\[ \text{do } i = 2, l_p - 1 \]
\[ k_2 = 0.5 \times (K_{Old}(i) + K_{Old}(i+1)) \]
\[ w_0(i) = cf_1 \times (k_2 \times (H_{Old}(i+1) - H_{Old}(i)) - k_1 \times (H_{Old}(i) - H_{Old}(i-1))) + Th_{Old}(i)/dt \]
\[ k_1 = k_2 \]
\[ \text{end do} \]

! first approximation of solution

\[ H_{Temp} = H_{Old} \]

\[ \text{call ComWater}(l_p, h_{Temp}, H_{Temp}, soil1) \]
\[ \text{call ComK}(l_p, h_{Temp}, K_{Temp}, soil1) \]

\[ \text{do } a = 0 \]
\[ b = 0 \]
\[ c = 0 \]
\[ w_1 = 0 \]
\[ k_1 = 0.5 \times (K_{Temp}(1) + K_{Temp}(2)) \]
\[ k_1n = 0.5 \times (K_{Temp}(1) + H_{Temp}(1) + Eps, soil1) + K_{Temp}(2) \]
\[ dq_1 = cf \times (k_1n \times (H_{Temp}(1) + Eps, soil1) - k_1 \times (H_{Temp}(1) - H_{Temp}(1))) - Th_{Temp}(1)/dt \]
\[ k_2 = 0.5 \times (K_{Temp}(1) + K_{Temp}(2)) \]
\[ w_1 = cf \times (k_2 \times (H_{Temp}(2) - H_{Temp}(1)) - k_1 \times (H_{Temp}(2) - H_{Temp}(1))) - Th_{Temp}(1)/dt \]
\[ k_3n = 0.5 \times (K_{Temp}(1) + H_{Temp}(1) + Eps, soil1) + K_{Temp}(2) \]
\[ dq_3 = cf \times (k_3n \times (H_{Temp}(1) - H_{Temp}(1)) - k_2 \times (H_{Temp}(1) - H_{Temp}(1))) - Th_{Temp}(1)/dt \]
\[ k_4n = 0.5 \times (K_{Temp}(1) + H_{Temp}(1) + Eps, soil1) + K_{Temp}(2) \]
\[ dq_4 = cf \times (k_4n \times (H_{Temp}(1) - H_{Temp}(1)) - k_2 \times (H_{Temp}(1) - H_{Temp}(1))) - Th_{Temp}(1)/dt \]
\[ \text{do } i = 2, l_p - 1 \]
\[ k_2 = 0.5 \times (K_{Temp}(i) + K_{Temp}(i+1)) \]
\[ w_1(i) = cf \times (k_2 \times (H_{Temp}(i+1) - H_{Temp}(i)) - k_1 \times (H_{Temp}(i) - H_{Temp}(i-1))) + Th_{Temp}(i)/dt \]
\[ k_1 = k_2 \]
\[ dq_1 = dq_3 \]
\[ dq_2 = dq_4 \]
\[ \text{end do} \]

! upper boundary condition

if (NBPoints > 0) then

! specified head

\[ \text{do } i = 1, NBPoints \]
\[ a(i) = 0 \]
\[ b(i) = 0 \]
\[ c(i) = 1 \]
\[ w_1(i) = h_{bound} - H_{Temp}(i) \]
\[ \text{end do} \]
else

! zero flux

\[ k_1 = 0.5 \times (K_{Old}(1) + K_{Old}(2)) \]
\[ w_0(1) = cf \times (-k_1 \times (H_{Old}(1) - H_{Old}(1))) + Th_{Old}(1)/dt \]
\[ k_1 = 0.5 \times (K_{Temp}(1) + K_{Temp}(2)) \]
\[ w_1(1) = cf \times (-k_1 \times (H_{Temp}(1) - H_{Temp}(1))) - Th_{Temp}(1)/dt \]
\[ k_2 = 0.5 \times (K_{Temp}(1) + K_{Temp}(2)) \]
\[ w_1 = cf \times (-k_2 \times (H_{Temp}(2) - H_{Temp}(1))) - Th_{Temp}(1)/dt \]
\[ k_3n = 0.5 \times (K_{Temp}(1) + H_{Temp}(1) + Eps, soil1) + K_{Temp}(2) \]
\[ dq_3 = cf \times (k_3n \times (H_{Temp}(1) - H_{Temp}(1)) - k_2 \times (H_{Temp}(1) - H_{Temp}(1))) - Th_{Temp}(1)/dt \]
\[ k_4n = 0.5 \times (K_{Temp}(1) + H_{Temp}(1) + Eps, soil1) + K_{Temp}(2) \]
\[ dq_4 = cf \times (k_4n \times (H_{Temp}(1) - H_{Temp}(1)) - k_2 \times (H_{Temp}(1) - H_{Temp}(1))) - Th_{Temp}(1)/dt \]
\[ c(i) = (F_{Theta}(H_{Temp}(1) - Eps, soil1) - Th_{Temp}(1))/Eps/dt/2 - dq_3 \]
\[ a(i) = 0 \]
\[ b(i) = -dq_4 \]
\[ w_2(i) = w_1(i) + w_0(i) \]
\[ k_1 = k_2 \]
\[ dq_1 = dq_3 \]
\[ dq_2 = dq_4 \]
\[ \text{end do} \]

! lower boundary condition

! zero flux

\[ k_1 = 0.5 \times (K_{Old}(lp-1) + K_{Old}(lp)) \]
\[ w_0(lp) = cf \times (-k_1 \times (H_{Old}(lp) - H_{Old}(lp))) + Th_{Old}(lp)/dt \]
\[ k_1 = 0.5 \times (K_{Temp}(lp-1) + K_{Temp}(lp)) \]
\[ w_1(lp) = cf \times (-k_1 \times (H_{Temp}(lp) - H_{Temp}(lp))) - Th_{Temp}(lp)/dt \]
\[ k_2 = 0.5 \times (K_{Temp}(lp-1) + K_{Temp}(lp)) \]
\[ w_1 = cf \times (-k_2 \times (H_{Temp}(lp) - H_{Temp}(lp))) - Th_{Temp}(lp)/dt \]
\[ k_3n = 0.5 \times (K_{Temp}(lp-1) + H_{Temp}(lp) + Eps, soil1) + K_{Temp}(lp) \]
\[ dq_3 = cf \times (k_3n \times (H_{Temp}(lp) - H_{Temp}(lp)) - k_2 \times (H_{Temp}(lp) - H_{Temp}(lp))) - Th_{Temp}(lp)/dt \]
\[ k_4n = 0.5 \times (K_{Temp}(lp-1) + H_{Temp}(lp) + Eps, soil1) + K_{Temp}(lp) \]
\[ dq_4 = cf \times (k_4n \times (H_{Temp}(lp) - H_{Temp}(lp)) - k_2 \times (H_{Temp}(lp) - H_{Temp}(lp))) - Th_{Temp}(lp)/dt \]
\[ c(lp) = (F_{Theta}(H_{Temp}(lp) - Eps, soil1) - Th_{Temp}(lp))/Eps/dt/2 + dq_3 \]
\[ a(lp) = dq_3 \]
\[ b(lp) = 0 \]
\[ w_2(lp) = w_1(lp) + w_0(lp) \]
end if

! checking for termination of iterations for macro equation

\[ \text{call Termin}(l_p, h_{Temp}, h_{New}, 0.25 \times Par\% AbsTol, 0.25 \times Par\% RelTol, endcalc) \]

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if (endcalc.or.(ni1>=par%NItMax)) exit

hTemp=hNew
ThTemp=ThNew
KTemp=KNew

end do !solution of macroscopic equation

if (ni1>par%bniter) par%bniter=ni1
par%btiter=par%btiter+ni1

! calculation of average water content
WCNew=0.
do i=1,lp-1
WCNew=WCNew+0.5*(ThNew(i)+ThNew(i+1))*dz
end do
WCNew=WCNew/((lp-1)*dz)
end subroutine Newton1D

!**************************************************************
subroutine Solve2DSolid(Maxbl,HBlockOld,HBlockNew,ThBlockOld,ThBlockNew,KBlockOld,KBlockNew,&
dblock,soil1,par,HBound,WCNew)
! solves the microscopic problem by decomposition of spatial
! operator
implicit none
integer maxbl

type (TSoilPar):: soil1
type (TMicroDis):: dblock
type (TMacroDis):: col_x,col_y
type (TNumPar):: par
real(8) HBlockOld(maxbl),HBlockNew(maxbl),&
ThBlockOld(maxbl),ThBlockNew(maxbl),&
KBlockOld(maxbl),KBlockNew(maxbl)
!
real(8),allocatable:: hc0(:),hct(:),&
tetc0(:),tetc1(:),kkc0(:),kkc1(:)
real(8) tet_s,dx,dy,dt,hbound,kb,tb,WCNew,ww
integer lx,ly,lx1,ly1,i,j,k,np
!
! initialization of variables
dt=par%dt
par%bniter=0
lx=dblock%lx1
ly=dblock%ly1
lx1=dblock%lx
ly1=dblock%ly
dx=dblock%dx
dy=dblock%dy
col_x%dz=dx
col_y%dz=dy
tb=FTheta(HBound,soil1)
k=FKh(HBound,soil1)
!
! introduction of boundary conditions
!
! first step - x dir.
! setting the values of boundary conditions
allocate(hc0(lx))
allocate(hct(lx))
allocate(tetc0(lx))
allocate(tetc1(lx))
allocate(kkc0(lx))
allocate(kkc1(lx))
!
! setting coefficients for x dir.
np=1+(j-1)*lx
hc0(i)=HBlockOld(np)
tetc0(i)=ThBlockOld(np)
kcc0(i)=KBlockOld(np)
end do
!
call Newton1d(lx,hc0,hct,tetc0,tetc1,kkc0,kkc1,&
par,col_x,soil1,hBound,1,ww)

! calculation in loop over y
!
do j=2,ly
do i=1,lx
!
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Appendix B. DPOR–1D source code

! setting initial condition for the second step
do i=1,lx
   HBlockNew(i)=hBound
   ThBlockNew(i)=tb
   KBlockNew(i)=kb
end do
!
! setting boundary conditions
allocate(hc0(ly))
allocate(hct(ly))
allocate(tetc0(ly))
allocate(tetc1(ly))
allocate(kkc0(ly))
allocate(kkc1(ly))
!
! calculation in loop over x
!
!
!


WcNew=0.
do i=1,lx-1
   do j=1,ly-1
      tet_s=ThBlockNew(i+(j-1)*lx)+ThBlockNew(i+(j-1)*lx)+ThBlockNew(i+j*lx)+ThBlockNew(i+1+j*lx)
      WCNew=WCNew+0.25*tet_s*dx*dy
   end do
end do
WcNew=WCNew/(0.25*dblock%IncX*dblock%IncY)
end subroutine Solve2DSolid

end subroutine Solve2DHollow

subroutine Solve2DHollow(MaxBl,HBlockOld,HBlockNew,ThBlockOld,ThBlockNew,KBlockOld,KBlockNew,&
Appendix B. DPOR–1D source code

dblock,soil1,par,HBound,WCNew)

! solves the microscopic problem by decomposition of spatial
! operator

implicit none

integer maxbl

type (TSoilPar):: soil1

type (TMicroDis):: dblock

type (TMacroDis):: col_x,col_y

type (TNumPar):: par

real(8) HBlockOld(maxbl),HBlockNew(maxbl),
     ThBlockOld(maxbl),ThBlockNew(maxbl),
     KBlockOld(maxbl),KBlockNew(maxbl)

!----------------------------------------------------------------------

real(8),allocatable:: hc0(:),hcp(:),hct(:),
     tetc0(:),tetc1(:),kkc0(:),kkc1(:)

real(8) tet_s,dx,dy,dt,hbound,kb,ww,wcnew

integer lx,ly,lx1,ly1,i,j,k,np

!--------------------------------------------------------------------
! initialization of variables
!do i=1, lx
! print *,h_blok0(i,6,6)
!end do
!read*

dt=par%dt
par%bniter=0

lx=dblock%lx
ly=dblock%ly
lx1=dblock%lx1
ly1=dblock%ly1

dx=dblock%dx
dy=dblock%dy
col_x%lp=lx
col_y%lp=ly
col_x%dz=dx
col_y%dz=dy

tb=FTheta(HBound,soil1)
kb=Fkh(HBound,soil1)

!----------------------------------------------------------------------
! introduction of boundary conditions
!----------------------------------------------------------------------
!
! first step - x dir.
! setting the values of boundary conditions
allocate(hc0(lx))
allocate(hct(lx))
allocate(tetc0(lx))
allocate(tetc1(lx))
allocate(kkc0(lx))
allocate(kkc1(lx))

! calculation in loop over y

do j=1,ly1
! setting coefficients for x dir.
np=i+(j-1)*lx
hc0(i)=HBlockOld(np)
tetc0(i)=ThBlockOld(np)
kkc0(i)=KBlockOld(np)
end do

call Newton1d(lx,hc0,hct,tetc0,tetc1,kkc0,kkc1,&
   par,col_x,soil1,hBound,lx1,ww)

do i=1, lx
np=1+(j-1)*lx
HBlockRev(np)=hct(i)
ThBlockRev(np)=tetc1(i)
end do

end do

end do

!
! setting coefficients for x dir.
!
end do

!

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end do
end do
!print *,'xxx'
deallocate(hc0)
deallocate(hct)
deallocate(tetc0)
deallocate(tetc1)
deallocate(kkc0)
deallocate(kkc1)

! setting initial condition for the second step
!
do i=1, lx1
    do j=1, ly1
        np=i+(j-1)*lx
        HBlockNew(np)=hbound
        ThBlockNew(np)=tb
        KBlockNew(np)=kb
    end do
end do
!
second step - y dir.
!
allocate(hc0(ly))
allocate(hct(ly))
allocate(tetc0(ly))
allocate(tetc1(ly))
allocate(kkc0(ly))
allocate(kkc1(ly))
!
! calculation in loop over x
!
do i=1,lx1
    do j=1,ly
        np=i+(j-1)*lx
        hc0(j)=HBlockNew(np)
        tetc0(j)=ThBlockNew(np)
        kkc0(j)=KBlockNew(np)
    end do
    call newton1d(ly,hc0,hct,tetc0,tetc1,kkc0,kkc1,&
                   par,col_y,soil1,hbound,ly1,ww)
    do j=1, ly
        np=i+(j-1)*lx
        HBlockNew(np)=hct(j)
        ThBlockNew(np)=tetc1(j)
        KBlockNew(np)=kkc1(j)
    end do
end do
end do
!
!!calculation in loop over x!!!
!
do i=1x1+1,lx
    do j=1,ly
        np=i+(j-1)*lx
        HBlockNew(np)=hct(j)
        ThBlockNew(np)=tetc1(j)
        KBlockNew(np)=kkc1(j)
    end do
end do
!
!print *,'yyy'
deallocate(hc0)
deallocate(hct)
deallocate(tetc0)
deallocate(tetc1)
deallocate(kkc0)
deallocate(kkc1)

! setting initial condition for the second step
!
do i=1, lx1
    do j=1, ly1
        np=i+(j-1)*lx
        HBlockNew(np)=hbound
        ThBlockNew(np)=tb
        KBlockNew(np)=kb
    end do
end do

WCNew=0.
do i=1,lx-1
    do j=ly1,ly-1
        tet_s=ThBlockNew(i+(j-1)*lx)+&
        ThBlockNew(i+1+(j-1)*lx)+&
    end do
end do

end do
end do

!print *,'yyy'
deallocate(hc0)
deallocate(hct)
deallocate(tetc0)
deallocate(tetc1)
deallocate(kkc0)
deallocate(kkc1)

! setting initial condition for the second step
!
do i=1, lx1
    do j=1, ly1
        np=i+(j-1)*lx
        HBlockNew(np)=hbound
        ThBlockNew(np)=tb
        KBlockNew(np)=kb
    end do
end do

WCNew=0.
do i=1,lx-1
    do j=ly1,ly-1
        tet_s=ThBlockNew(i+(j-1)*lx)+&
        ThBlockNew(i+1+(j-1)*lx)+&
    end do
end do

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Appendix B. DPOR–1D source code

end subroutine Solve2DHollow

!******************************************************************************
subroutine Solve3D(maxbl,HBlockOld,HBlockNew,ThBlockOld,ThBlockNew,KBlockOld,KBlockNew,&
dblock,soil1,par,HBound,WCNew,NNB,NBound)
! solves the microscopic problem by decomposition of spatial
! operator
implicit none
integer maxbl
type (TSoilPar):: soil1
type (TMicroDis):: dblock
type (TNumPar):: par
real(8) HBlockNew(maxbl),HBlockOld(maxbl),&
ThBlockOld(maxbl),ThBlockNew(maxbl),&
KBlockOld(maxbl),KBlockNew(maxbl)
!----------------------------------------------------------------------
! initialization of variables
!----------------------------------------------------------------------
t=par%t
dt=par%dt
par%bniter=0
lx=dblock%lx
ly=dblock%ly
lb=dblock%lz
dx=dblock%dx
dy=dblock%dy
dz=dblock%dz
col_x%lp=lx
col_y%lp=ly
col_z%lp=lb
col_x%dz=dx
col_y%dz=dy
col_z%dz=dz
col_x%dz=dx
col_y%dz=dy
col_z%dz=dz
col_x%len=dblock%IncX/2.
col_y%len=dblock%IncY/2.
col_z%len=dblock%IncZ/2.
tb=FTheta(hBound,soil1)
kb=FKh(hBound,soil1)
!--------------------------------------------------------------------
! introduction of boundary conditions
!-----------------------------------------------------------------------
! first step - x dir.
! allocating arrays
allocate(hc0(lx))
allocate(hct(lx))
allocate(tetc0(lx))
allocate(tetc1(lx))
allocate(kkc0(lx))
allocate(kkc1(lx))
! calculation in loop over y and z
do j=2,ly
  do k=2,lz
    do i=1,tx
      ! setting coefficients for x dir.
      np=i+(j-1)*lx+(k-1)*lx*ly
      hc0(i)=HBlockOld(np)
tetc0(i)=ThBlockOld(np)
tetc1(i)=ThBlockOld(np)
kkc0(i)=KBlockOld(np)
kkc1(i)=KBlockOld(np)
      end do
      call Newton1d(lx,hc0,hct,tetc0,tetc1,kkc0,kkc1,&
                  par,col_x,soil1,hBound,1,ww)
    end do
  end do
end do

!******************************************************************************

do i=1, lx
  np=i+(j-1)*lx+(k-1)*lx*ly
  HBlockNew(np)=hct(i)
  ThBlockNew(np)=tetc1(i)
  KBlockNew(np)=kkc1(i)
end do
end do
end do
!print *, 'xxx'
deallocate(hc0)
disable(hct)
deallocate(tetc0)
deallocate(tetc1)
deallocate(kkc0)
deallocate(kkc1)

!-----------------------------------------------------------------
! setting initial condition for the second step
!-----------------------------------------------------------------
! second step - y dir.
! setting boundary conditions
allocate(hc0(ly))
allocate(hct(ly))
allocate(tetc0(ly))
allocate(tetc1(ly))
allocate(kkc0(ly))
allocate(kkc1(ly))
!-----------------------------------------------------------------
! calculation in loop over x and z
!-----------------------------------------------------------------
! third step - z dir.
! setting boundary condition
allocate(hc0(lz))
allocate(hct(lz))
allocate(tetc0(lz))
allocate(tetc1(lz))
allocate(kkc0(lz))
allocate(kkc1(lz))
! calculation in loop over x and y
!-----------------------------------------------------------------

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end do
end do
end do
!print *,’zzz’nend do
deallocate(hc0)
deallocate(hct)
deallocate(tetc0)
deallocate(tetc1)
deallocate(kkc0)
deallocate(kkc1)

!--------------------------------------------------------------
do i=1, NNB
HBlockNew(NBound(i))=hBound
KBlockNew(NBound(i))=kb
ThBlockNew(NBound(i))=tb
end do
!------------------------------------------------------------
WcNew=0.
do i=1,lx-1
do j=1,ly-1
do k=1,lz-1
np=i+(j-1)*lx+(k-1)*lx*ly
tet_s=ThBlockNew(np)+ThBlockNew(np+1)+ThBlockNew(np+lx)+ThBlockNew(np+lx+1)+ThBlockNew(np+lx*ly)+ThBlockNew(np+1+lx*ly)+ThBlockNew(np+lx+lx*ly)+ThBlockNew(np+1+lx+lx*ly)
WCNew=WCNew+0.125*tet_s*dx*dy*dz
end do
end do
end do
WCNew=WCNew/(0.125*dblock%IncVol)
end subroutine Solve3D

!************************************************************************
subroutine SolveSphere(maxdir,hOld,hNew,ThOld,ThNew,KOld,KNew,&
par,dblock,soil,HBound,WcNew,rr)
implicit none
integer maxdir
type (TSoilPar):: soil
type (TMicroDis):: dblock
type (TNumPar):: par
real(8) HOld(maxdir),HNew(maxdir),HTemp(maxdir),w0(maxdir),w1(maxdir),dh(maxdir),&
a(maxdir),b(maxdir),c(maxdir),ThNew(maxdir),KNew(maxdir),&
ThOld(maxdir),KOld(maxdir),ThTemp(maxdir),KTemp(maxdir),rr(maxdir),&
k1,k2,hbt,hbb,t,dt,dz,beta,cf,cf1,hbound,qb,wcNew
integer i,j,lp,lk,ni1
logical endcalc
lp=dblock%lx
dt=par%dt
dz=dblock%dx
beta=par%beta
par%bniter=0
cf=(1.-beta)/dz/dz*dt
cf1=beta/dz/dz*dt
w0=0.
k1=0.5*(KOld(1)+KOld(2))
do i=2,lp-1
k2=0.5*(KOld(i)+KOld(i+1))
w0(i)=cf*(k2*(hOld(i+1)-hOld(i))-k1*(hOld(i)-hOld(i-1)))+FTheta(hOld(i),soil)&
+cf/rr(i)*dz*(k2*(hOld(i+1)-hOld(i))+k1*(hOld(i)-hOld(i-1)))
k1=k2
end do
! first approximation of the solution
Appendix B. DPOR-1D source code

hTemp=hOld
call ComWater(lp,HTemp,ThTemp,soil)
call ComK(lp,HTemp,KTemp,soil)
do
  a=0
  b=0
  c=0
  w1=w0
  k1=0.5*(KTemp(1)+KTemp(2))
do i=2,lp-1
    k2=0.5*(KTemp(i)+KTemp(i+1))
    a(i)=-k1*cf1+k1*cf1*dz/rr(i)
    b(i)=-k2*cf1-k2*cf1*dz/rr(i)
    c(i)=FCap(hTemp(i),soil)+(k1+k2)*cf1*(k2-k1)+cf1*dz/rr(i)
    w1(i)=w1(i)+cf1*(k2*(HTemp(i+1)-HTemp(i))-k1*(HTemp(i)-HTemp(i-1)))-FTheta(HTemp(i),soil)
    +cf1*dz/rr(i)*(k2*(HTemp(i+1)-HTemp(i)))*k1*(HTemp(i)-HTemp(i-1))
  end do
  k1=k2
end do

! upper boundary condition
  a(lp)=0.
  b(lp)=-1.
  c(lp)=1.
  w1(lp)=HTemp(2)-HTemp(1)

! lower boundary condition
! head
  a(lp)=0.
  b(lp)=0.
  c(lp)=1.
  w1(lp)=hbound-HTemp(1p)
call Thomas(lp,a,b,c,w1,dh)

HNew=HTemp+dh
call ComWater(lp,HNew,ThNew,soil)
call ComK(lp,HNew,KNew,soil)
par%bniter=par%bniter+1
call termin(lp,HTemp,HNew,0.25*par%AbsTol,0.25*par%RelTol,endcalc)
if (endcalc.or.(par%bniter>=par%NItMax)) exit
  Htemp=hNew
  ThTemp=ThNew
  KTemp=KNew
end do

par%btiter=par%btiter+par%bniter

! calculation of transfer term
WCNew=0.
do i=1,lp-1
  WCNew=WCNew+0.5*(ThNew(i)+ThNew(i+1))
  *(4./3.*pi*(rr(i+1)**3.-rr(i)**3.))
end do
WCNew=WCNew/(4./3.*pi*rr(lp)**3.)
end subroutine SolveSphere

subroutine SolveCylinder(maxdir,hOld,hNew,ThOld,ThNew,KOld,KNew,&
                        par,dblock,soil,HBound,WcNew,rr)
  implicit none
  integer maxdir
  type (TSoilPar):: soil
  type (TMicroDis):: dblock
  type (TNumPar):: par
  real(8) HOld(maxdir),HNew(maxdir),HTemp(maxdir),w0(maxdir),w1(maxdir),dh(maxdir),&
         a(maxdir),b(maxdir),c(maxdir),ThNew(maxdir),KNew(maxdir),&
         ThOld(maxdir),KOld(maxdir),ThTemp(maxdir),rr(maxdir),&
         k1,k2,hbt,hbb,t,dt,dz,beta,cf,cf1,hbound,qb,wcNew
  integer i,j,lp,lk,ni1
  logical endcalc
  lp=dblock%lx
dt=par%dtd
dz=dblock%dx
  beta=par%beta
  par%bniter=0
  cf=(1.-beta)/dz/dz*dt
  cf1=beta/dz/dz*dt
  w0=0.
Appendix B. DPOR–1D source code

```plaintext
k1=0.5*(KOld(1)+KOld(2))
do i=2,lp-1
  k2=0.5*(KOld(i)+KOld(i+1))
  w0(i)=cf*(k2*(hOld(i+1)-hOld(i))-k1*(hOld(i)-hOld(i-1)))+FTheta(hOld(i),soil) &
         +0.5*cf/rr(i)*dz*(k2*(hOld(i+1)-hOld(i))+k1*(hOld(i)-hOld(i+1)))
  k1=k2
end do

! first approximation of the solution
hTemp=hOld
call ComWater(lp,HTemp,ThTemp,soil)
call ComK(lp,HTemp,KTemp,soil)
do
  a=0
  b=0
  c=0
  w1=w0
  k1=0.5*(KTemp(1)+KTemp(2))
do i=2,lp-1
    k2=0.5*(KTemp(i)+KTemp(i+1))
    c(i)=FCap(hTemp(i),soil)+(k1+k2)*cf1+(k2-k1)*0.5*cf1*dz/rr(i)
    a(i)=-k1*cf1+0.5*k1*cf1*dz/rr(i)
    b(i)=-k2*cf1-0.5*k2*cf1*dz/rr(i)
    w1(i)=w1(i)+cf1*(k2*(HTemp(i+1)-HTemp(i))-k1*(HTemp(i)-HTemp(i-1)))-FTheta(HTemp(i),soil) &
          +0.5*cf1*dz/rr(i)*(k2*(HTemp(i+1)-HTemp(i))+k1*(HTemp(i)-HTemp(i+1)))
  k1=k2
end do

! upper boundary condition
a(1)=0.
b(1)=1.
c(1)=1.
w1(1)=HTemp(2)-HTemp(1)

! lower boundary condition
!head
a(lp)=0.
b(lp)=0.
c(lp)=1.
w1(lp)=hbound-HTemp(lp)
call Thomas(lp,a,b,c,w1,dh)
HNew=HTemp+dh
call ComWater(lp,HNew,ThNew,soil)
call ComK(lp,HNew,KNew,soil)
call termin(lp,HTemp,HNew,0.25*par%AbsTol,0.25*par%RelTol,endcalc)
if (endcalc.or.(par%bniter>=par%NItMax)) exit

HTemp=HNew
ThTemp=ThNew
KTemp=KNew
par%bniter=par%bniter+1
par%btiter=par%btiter+par%bniter

! calculation of transfer term
WCNew=0.
do i=1,lp-1
  WCNew=WCNew+0.5*(ThNew(i)+ThNew(i+1))&
         *(pi*(rr(i+1)**2.-rr(i)**2.))
end do
WCNew=WCNew/(pi*rr(lp)**2.)

end subroutine SolveCylinder
!*****************************************************************************
end module MicSolv
```

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Abstract

The thesis concerns the unsaturated water flow in soils composed of two distinct sub-domains with contrasting hydraulic parameters (double-porosity soils). The analysis start at the Darcy scale, where the flow in each sub-domain is described by the Richards equation. The asymptotic homogenization method is used to derive macroscopic models for two types of soil structure, i.e. with weakly conductive and highly conductive inclusions. In each case one obtains a one-equation nonlinear model arises. The effective conductivity of the medium is calculated from the local boundary value problem and it is independent of the conductivity of inclusions. For the soil with weakly conductive inclusions the macroscopic model has non-equilibrium character and contains an integral term, which represents the exchange of water between the two sub-domains. The obtained models are compared to other approaches existing in literature. The models are implemented into a numerical code DPOR-1D. It enables the simulation of macroscopically 1D flow in soils with various geometries of 2D and 3D inclusions (circle, rectangle, sphere, parallelepiped). The results obtained with DPOR-1D code are close to the fine scale numerical solution, where the heterogeneous structure of the medium is explicitly represented. The DPOR-1D simulations are also in good agreement with the results of 1D infiltration experiments in a 60-cm long vertical column filled with a mixture of sand and sintered clayey spheres.

Résumé

La thèse concerne l’écoulement insaturé d’eau dans les sols composés de deux régions distinctes aux paramètres hydrodynamiques contrastés (sols à double porosité). Le point de départ de l’analyse est la description de l’écoulement à l’échelle de Darcy (équations de Richards). La méthode d’homogénéisation par développements asymptotiques est utilisée pour dériver les modèles macroscopiques pour deux structures différentes: sols avec des inclusions plus conductrices ou moins conductrices par rapport à la matrice. Pour chaque structure un modèle macroscopique à une équation est obtenu. On montre, que la conductivité effective ne dépend pas de celle des inclusions. Elle est définie par la solution d’un problème aux limites local. Pour les sols avec des inclusions faiblement conductrices, un modèle de non équilibre local est obtenu, avec un terme intégral représentant l’échange d’eau entre les inclusions et la matrice. Les modèles développés sont ensuite comparés à d’autres approches de la littérature. Les modèles sont implémentés dans un code de calcul DPOR-1D, qui permet la modélisation d’écoulement macroscopiquement 1D pour des différentes géométries 2D ou 3D des inclusions (cercle, rectangle, sphère, parallélépipède). Les résultats obtenus avec DPOR-1D sont voisins de la solution numérique à l’échelle fine où la structure hétérogène du milieu est représentée explicitement. Les simulations numériques sont en bon accord avec les résultats d’expérimentations d’infiltration 1D dans une colonne verticale de 60 cm remplie par un mélange de sable et de billes d’argile solidifiée.

Streszczenie

Tematem pracy jest modelowanie przepływu wody w gruntach nienasyconych o podwójnej porowatości, które charakteryzują się obecnością dwóch podobszarów porowatych o skontrastowanych parametrach hydraulicznych. Jako punkt wyjścia przyjęto, że w skali lokalnej przepływ w obu podobszarach jest opisany równaniem Richardsa. Przedstawiono wypracowanie dwóch modeli przepływu w skali makroskopowej przy użyciu metody homogenizacji asymptotycznej. Modele te dotyczą odpowiednio gruntu z inkluzjami słabo przepuszczalnymi oraz z inkluzjami silnie przepuszczalnymi. Dla każdego z tych przypadków otrzymano model w formie pojedynczego równania nieliniowego. Efektywny współczynnik przewodności jest zdefiniowany poprzez rozwiązanie lokalnego problemu brzegowego w pojedynczym elemencie reprezentatywnym. Współczynnik ten nie zależy od przewodności inkluzji. Dla gruntu z inkluzjami słabo przpuszczalnymi otrzymano model z dodatkowym członem całkowym, opisującym wymianę wody między dwoma podobszarami (model lokalnej nierównowagi ciśnienia). Otrzymane modele porównano z innymi, istniejącymi w literaturze. Modele zostały zaimplementowane w programie DPOR-1D. Program umożliwia symulację przepływu makroskopowo jednowymiarowego z uwzględnieniem dwu- lub trójwymiarowej geometrii inkluzji (koło, prostokąt, kula, prostopadłościan). Otrzymane wyniki są zgodne z rozwiązaniem numerycznym w skali lokalnej, w którym niejednorodna struktura gruntu jest uwzględniona w sposób jawny. Symulacje numeryczne programem DPOR-1D są również zbliżone z wynikami eksperymentalnymi (infiltracja w kolumnie o wysokości 60 cm, wypełnionej mieszaniną piasku i kulek z wypalonej gliny).