Determinaton of constitutive relationships for two–phase flow processes in heterogeneous porous media with emphasis on the relative permeability–saturation–relationship

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Abstract

Assessment of contaminations by dense non–aqueous phase liquids (DNAPL) and their remediation often requires numerical simulations on the macroscale. Effective parameters for the macroscale are required for these simulations in order to avoid a detailed discretisation of the geological structures. Starting from the observed influence of heterogeneities on multiphase flow processes on the macroscale, we present an upscaling procedure from the local to the macroscale for the derivation of constitutive relationships for multiphase flow processes. The approach is based on the assumption of an equilibrium of (capillary) forces, which allows the application of a percolation model. This results in saturation distributions for different capillary pressures. Averaging these distributions gives rise to a macroscopic capillary pressure–saturation–relationship. For the saturation distribution relative permeabilities and effective conductivities are computed depending on the structure and the flow direction. These are averaged with the help of the renormalisation method. The evolving relative permeability–saturation – relationship for the macroscale shows a saturation dependent anisotropy and pronounced residual saturations of the non-wetting phase (which were not assumed for the local scale). The anisotropy reflects the underlying structure of the considered system which needs not to be known in detail.

Key words: two–phase flow, upscaling, averaging effective conductivity, saturation dependent anisotropy, macroscopic residual saturation
This contribution examines the conceptualisation of two–phase flow processes on the macroscale, as needed for the simulation of the surroundings of subsurface contaminations by organic solvents. Many numerical and experimental studies have shown that even heterogeneities on a centimetre–scale can dominate multiphase flow. To overcome the impossibility of collecting all the information about the geological heterogeneities on the small scale and of representing them discretely in the numerical model upscaled, effective parameters can be employed. These should represent the influence of the lower scale heterogeneities on two-phase flow behaviour on the scale on which the simulation takes place. For two–phase flow processes such effective parameters could be the constitutive relationships, namely the capillary pressure–saturation–relationship ($P_c - S_w$) and the relative permeability–saturation–relationship ($k_r - S$). Consequently, these need to be upscaled consistently.

The first upscaling step goes from the pore scale to the local scale (see Figure 1). It results in a set of parameters for each material for which an REV can be determined. The next scale transition takes us from the local scale to the macro scale (see Figure 1). In this paper we will concentrate on the upscaling of saturation–dependent parameters for this scale transition. Thus the upscaling procedure should take into account the local scale constitutive relationships and information about the structure of the geological system under consideration as far as both are known. For the calculation of the relative permeability–saturation–relationship, e.g., we will present an approach that allows to average a saturation dependent anisotropic relation from the local to the macroscale which represents the influence of the geological heterogeneities of the local scale on the macroscale.

The paper is mainly concerned with two–phase flow processes that are relevant to contaminations by dense non–aqueous phase liquids (DNAPL), such as organic solvents, in heterogeneous subsurface systems. For the assessment of these flow processes, two variables are mainly of interest: saturations and fluxes. This will be taken into account when we develop our upscaling approach.

To gain a better understanding of the main processes and assumptions, we will first identify the dominant parameters on the scales of interest and the relevant processes in a heterogenous system on the macroscale. Different upscaling methods developed in the past will be presented, in a search for one which accounts for the dominating forces and the relevant flow processes. The focus here lies on the reduction of variables by assuming an equilibrium of (capillary) forces. This assumption leads to the application of a percolation model which, together with the renormalisation as one averaging method, results in effective
constitutive relationships for the macroscale.

This approach thus allows us to derive effective parameters for the enhanced simulation of two–phase flow in heterogeneous porous media on the macroscale. The results of the application of this upscaling approach show that it is questionable to use the same constitutive relationships for the upscaling from the local to macroscale as for the upscaling from the porescale to the local scale.

One advantage of the approach is its easy applicability. Furthermore, its physical motivation facilitates a physical interpretation of the upscaled parameters, which are saturation dependent. At the end of the paper, the effective parameters thus derived are verified with the simulation of a bench scale laboratory experiment.

1.1 Physical and mathematical model on different scales

In the theory of porous media, the smallest scale considered is usually the pore scale (see Figure 1). On this scale, the density and the viscosity have already been averaged starting from the molecular scale. These fluid properties are invariant on the subsequent higher scales.

Fig. 1. Definition of scales

On the pore scale, the two–phase flow processes are predominantly influenced by the pore geometry. On the subsequent larger scale, the local scale, the equations for the conservation of mass and momentum can be derived by volume averaging over the pore scale properties, applying the concept of the REV [5]. A large number of multiphase experiments has proven that the velocity for each phase in a porous medium can be described by the generalised Darcy’s law [37]. In the course of the averaging procedure from the pore to the local scale, new variables appear. In a multiphase system, this is, for example, the saturation. Regarding the influence of the porous medium, the permeability appears
on the local scale. In a porous medium with two–phases, the strongest forces on the local scale at typical flow velocities, are the interfacial forces. Thus, the capillary pressure–relative permeability–saturation–relationship can be considered the most important characteristic on the local scale [30], as it accounts for the interaction between multiple fluids and the porous medium.

Within the scope of this paper, the following assumptions are made on the local scale for the conservation of mass and momentum:

(1) Darcy’s law holds for the conservation of momentum in two–phase flow processes.
(2) The relations of saturation, capillary pressure, and relative permeability are described by the common parametrisations after Van Genuchten / Mualem [23, 32] and Brooks & Corey / Burdine [10, 11, 15]. Hysteresis and residual saturations are not considered on the local scale. In this paper we will only apply the constitutive relationships after Brooks & Corey / Burdine. Any other constitutive relationships can be easily substituted in the upscaling procedure. Possible dynamic effects [22] or further functional dependencies, e.g. on the interfacial area [13], are also neglected.
(3) The porous medium is assumed to be isotropic on the local scale. Thus, the intrinsic permeability and relative permeability–saturation–relationship are scalar functions.
(4) Both the porous medium and the fluids are incompressible.

Mathematically, the conservation of mass and momentum on the continuum scale are combined to [24]:

\[
\text{div} \left( \frac{1}{\mu_w} k_{rw} K_0 \cdot (\text{grad} (P_w) - \rho_w g) \right) - \rho_w q_w = - \phi \frac{\partial (S_w)}{\partial t},
\]

(1)

\[
\text{div} \left( \frac{1}{\mu_n} k_{rn} K_0 \cdot (\text{grad} (P_n) - \rho_n g) \right) - \rho_n q_n = - \phi \frac{\partial (S_n)}{\partial t}.
\]

(2)

These two partial differential equations are coupled by the restrictions that the saturations must add up to one and that the gradient of the capillary pressure can be defined as:

\[
\text{grad} (P_c) = \text{grad} (P_n) - \text{grad} (P_w).
\]

(3)

Equations (1) and (2) are applied on the local scale. Yet, as mentioned before, an increased space scale might induce a change of the dominant processes and forces. The effective parameters, as will be derived here for the macroscale, should account for the varying influences. As a consequence, the mass and
momentum conservation equations might look different on the macroscale, e.g. the relative permeability–saturation–relationship might no longer be a scalar function but might depend on the direction.

In the next section a simple model problem will illustrate the effects of the interaction of the different parameters in a multiphase system.

1.2 Influence of Heterogeneities on Two Phase Flow

Multiphase systems in porous media are characterised by parameters such as the capillary pressure–relative permeability–saturation relationship. We will show the impact of the different parameters on the basis of a DNAPL infiltration process. Figure 2 shows the model domain with its boundary conditions. A DNAPL with a density that is 1.46 times higher than that of water and a viscosity of $\mu = 0.57 \cdot 10^{-3} \text{kg/(m \cdot s)}$ infiltrates from above into a heterogeneous domain, which is initially fully saturated with water. For simplicity’s sake the system is symmetric.

![Fig. 2. 2D model domain with boundary and initial conditions](image)

By varying the parameters of the lenses within for coarse sand to be expected deviances (see Table 1) we can examine the influence of each parameter separately. This is accomplished by neglecting any correlations of the parameters. The heterogeneous cases 2 to 5 will be compared directly to the homogeneous case 1 (see Figures 3 to 6).

Figure 3 shows the small impact of the porosity on the two–phase flow behaviour. The infiltration process is slightly accelerated for obvious reasons.

The influence of a reduced intrinsic permeability is much higher (see Figure 4). As the flow velocity is smaller in the lenses than in the background material, DNAPL pools up on the lenses to some extent and flows around them. Thus,
Table 1
Parameters of the lenses and the background material for the motivation example

<table>
<thead>
<tr>
<th></th>
<th>porosity</th>
<th>intrinsic permeability</th>
<th>entry pressure</th>
<th>form factor</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\phi$ [-]</td>
<td>$k_0$ [m$^2$]</td>
<td>$P_D$ [Pa]</td>
<td>$\lambda$ [-]</td>
</tr>
<tr>
<td>background material</td>
<td>0.4</td>
<td>$1.0 \cdot 10^{-10}$</td>
<td>1000</td>
<td>2</td>
</tr>
<tr>
<td>lenses, case 1</td>
<td>0.4</td>
<td>$1.0 \cdot 10^{-10}$</td>
<td>1000</td>
<td>2</td>
</tr>
<tr>
<td>lenses, case 2</td>
<td>0.3</td>
<td>$1.0 \cdot 10^{-10}$</td>
<td>1000</td>
<td>2</td>
</tr>
<tr>
<td>lenses, case 3</td>
<td>0.4</td>
<td>$1.0 \cdot 10^{-11}$</td>
<td>1000</td>
<td>2</td>
</tr>
<tr>
<td>lenses, case 4</td>
<td>0.4</td>
<td>$1.0 \cdot 10^{-10}$</td>
<td>$\sqrt{10} \cdot 1000 (\approx 3162)$</td>
<td>2</td>
</tr>
<tr>
<td>lenses, case 5</td>
<td>0.4</td>
<td>$1.0 \cdot 10^{-10}$</td>
<td>1000</td>
<td>4</td>
</tr>
</tbody>
</table>

Fig. 3. Distribution of $S_n$ (DNAPL) after 7 min, left hand side: case 1 (homogeneous reference), right hand side: case 2 (lenses with reduced porosity)

the main direction of the flow is diverted from the vertical to the horizontal direction.

This effect can also be observed when the entry pressure of the lenses, is increased compared to the background material (see Figure 5). Before the nonwetting phase can infiltrate into lenses the entry pressure of the lenses has to be overcome. This causes the pooling up of the DNAPL above the lenses and a horizontal flow.

Increasing the Brooks–Corey parameter $\lambda$ has two effects. On the one hand, it reduces the relative permeability of the nonwetting phase which causes a pooling–up of DNAPL on the lenses and an increased flow in the horizontal direction.

On the other hand, an increased $\lambda$ results in a capillary pressure–saturation...
curve with a more shallow slope than the curve of the background material. This results in a higher DNAPL saturation in the lenses at the same capillary pressure. The two effects cancel one another out so that the result that does not appear very different from the homogeneous case.

In summary, the intrinsic permeability and the entry–pressure conditions have the most distinct influence on the two–phase flow behaviour on the local to macroscale.

Now that the dominant parameters and processes have been identified, methods for the upscaling procedure have to be found. The chosen method should account for the dominant processes and forces and should also take the variables one is interested in into consideration. To describe the two–phase flow
Fig. 6. Distribution of $S_n$ (DNAPL) after 7 min; left-hand side: case 1 (homogeneous reference), right-hand side: case 5 (lenses with increased form factor $\lambda$)

processes occurring in the surrounding of groundwater contaminations with DNAPLs, it is preferable to represent the correct saturation distributions and integral fluxes, rather than, for example the displacement velocity as in the case of single-phase – multicomponent flow problems.

In the following, different upscaling techniques will be summarised and one appropriate for our field of application chosen.

1.3 Upscaling Methods

Many methods for deriving effective parameters on the macroscale can be found in the literature. They can be classified as follows:

- The *a posteriori–method* uses a highly resolved computation or measurement to analyse the flow processes. Effective parameters are derived from this analysis [14, 16]. A disadvantage of this method is the time-consuming simulation for the highly resolved domain. It is mainly applied in the petroleum industry.
- The application of *stochastic methods* requires assumptions about the statistical distribution of the heterogeneities. Effective parameters are calculated by stochastic averaging of the equations (e.g. [17, 31, 44, 45, 46]). The heterogeneity field and the correlation of the parameters have to satisfy certain requirements, which restricts the applicability of the method.
- For simple geometries, *analytical solutions* for the calculation of effective parameters can be found, for example, volume averaging (e.g. [1, 35, 36]).
- By means of the *analogy method*, upscaling–approaches from other scopes of research (e.g. transport problems in single phase flow) are transferred to two-phase flow applications (e.g. [33, 34, 43]).
Furthermore, the equilibrium method allows us to simplify the treated system, assuming an equilibrium of forces [6, 7, 33, 34, 43]. This is a common approach for reducing the number of variables.

The assumption of an equilibrium of capillary forces was applied especially to percolation models [29, 47]. Green et al. [21] thus computed averaged capillary pressure–saturation–relationships.

The advantages are the efficiency and the flexibility of the method. Our main reason for choosing the equilibrium of capillary forces together with a percolation model is the physical motivation of the approach. This facilitates the interpretation of the derived effective parameters.

2 Capillary Equilibrium

We apply the method of an equilibrium of forces to two–phase flow problems and make the following assumptions:

- As to the common model concepts we neglect dynamic effects which may have an influence on the determination of the constitutive relationships [22]. This premise already holds for the definition of the constitutive relationships on the local scale.
- Sources or sinks do not occur.
- Stationarity is presumed. Thus the parameters are averaged taking stationary problems. Nevertheless they might then be applied to transient processes. This is usually also done when determining the capillary pressure–saturation–relation under static conditions in the laboratory. These relations are then applied for the simulation of transient processes.

As the time derivatives and the source–sink terms vanish, the multiphase mass and momentum conservation equations (1) and (2) based on the $P_w - S_n$ formulation simplify to

\[ \text{div} \left( \frac{1}{\mu_w} k_{rw} K_0 \cdot (\text{grad} (P_w) - \rho_w g) \right) = 0, \]  \hspace{1cm} (4)

\[ \text{div} \left( \frac{1}{\mu_n} k_{rn} K_0 \cdot (\text{grad} (P_w) + \text{grad} (P_c) - \rho_n g) \right) = 0. \]  \hspace{1cm} (5)

Appropriate boundary conditions have to be found for these partial differential equations to ensure correct and unique upscaled variables. Different boundary
conditions will be applied to a simple horizontal 1D problem (see Figure 7) to show their influence.
Despite the entry pressure all the parameters of the materials are the same used for the background material of the motivation example (see Table 2). In this example, the dynamic viscosities of both fluid phases are set to \( \mu = 0.001 \text{ kg/(m} \cdot \text{s)} \).

With this numerical "Darcy" experiment, the effective conductivity for the whole domain can be computed by converting the Darcy equation:

\[
\bar{k} = \frac{q^m \cdot g \cdot L}{\Delta P \cdot A} \quad (6)
\]

First of all, cases one and two will be described. The applied flux boundary condition on the right hand side induces a flow of the wetting phase from the left to the right (case one) or from the right to the left (case two). In single phase flow situations, these boundary conditions would result in a unique value for the effective conductivity. However, in a two-phase flow problem additional degrees of freedom exist. Thus, boundary conditions have to be applied not only for the water but also for the nonwetting phase. A saturation of the nonwetting phase \( S_n = 0.6 \) induces a capillary pressure of \( P_c = 1581 \text{ Pa} \) on the left hand side and of \( P_c = 2371 \text{ Pa} \) on the right hand side (see Figure 8). As the pressures have to have a continuous progression over the domain, a capillary pressure gradient evolves, whose direction is fixed.

In Figure 9 the trends of the variables \( P_w, P_c, S_w, k_r \) are shown for the different cases. None of the courses of the curves is linear. As mentioned above, the boundary conditions induce a capillary pressure gradient. The course of the curve of the saturation and relative permeability curve at the transition of the heterogeneity depends on the discretisation, in an ideal system this would be a sharp interface.

Because of the nonlinearity of the capillary pressure–saturation–relationship the resulting saturations are not constant and do not possess a uniform
Fig. 9. Trends of the variables $P_w, P_c, S_w, k_r$ for cases 1 and 2

gradient. Variable saturations also produce variable relative permeabilities. However, the constant flux (boundary condition) must be proportional to the relative permeability and the pressure gradient (see Equation 6). Thus, in the case of variable relative permeabilities, the pressure gradient has to be nonlinear to ensure a constant flux.

Moreover, the pressure differences which evolve in case one and two differ (see Table 3). The two partial differential equations (4) and (5) are coupled by the restriction $\text{grad } (P_w) = \text{grad } (P_h) - \text{grad } (P_c)$. In the first case, the gradient of the capillary pressure points in the direction opposite that of the flow whereas, in the second case the gradient of the capillary pressure points into the same direction. Thus different pressure gradients of the water phase and different saturations evolve. This effect is reinforced by the nonlinearity of the constitutive relationships.

This example shows that, with the boundary conditions chosen as above, a heterogeneous two-phase flow system does not possess a unique effective conductivity. If we choose different boundary conditions, we can induce an equilibrium of forces. This is achieved by applying the same capillary pressure at
Table 3
Pressure differences and hydraulic conductivities for the four cases

<table>
<thead>
<tr>
<th>case 1</th>
<th>case 2</th>
<th>case 3</th>
<th>case 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta P_w$ [Pa]</td>
<td>701</td>
<td>377</td>
<td>23</td>
</tr>
<tr>
<td>$K$ [m/s]</td>
<td>$1.40 \cdot 10^{-5}$</td>
<td>$2.60 \cdot 10^{-5}$</td>
<td>$4.27 \cdot 10^{-4}$</td>
</tr>
</tbody>
</table>

the boundaries (see Table 2). This effects a constant capillary pressure and in correlation to that a piecewise constant saturation distribution, which causes a piecewise constant relative permeability distribution. Then, the only degree of freedom is the pressure gradient of the wetting phase. Accordingly, a unique effective conductivity can be computed, stationarity always presumed (see Table 3). Assuming this kind of (equilibrium) boundary conditions the averaging procedure of conductivities for the two–phase flow system is similar to that well known from single phase flow.

Fig. 10. Trends of the variables $P_w$, $P_c$, $S_w$, $k_r$ for the cases 3 and 4 of the capillary equilibrium example

This example has proven that, with the assumption of a capillary equilibrium, it is possible to define unique effective conductivities in a heterogeneous, two–phase system. The capillary equilibrium ensures a constant saturation and
relative permeability distribution for stationary problems, allowing the derivation of unique effective conductivities. Consequently, we will use the restriction of capillary equilibrium on the boundary conditions in the following to derive effective parameters.

3 Description of the Upscaling Approach

In this section, we will describe the different methods that comprise the proposed upscaling approach, used to derive effective parameters on the macroscale for the simulation of two-phase flow processes.

Starting from the local scale we have to determine the distribution of all material parameters and constitutive relationships (see Figure 11). Applying the capillary equilibrium assumption to a distribution of local $P_c - S_w$ relationships we can determine the saturation distribution for a given capillary pressure. In this paper we will first focus on simple geometric structures of heterogeneities. In that case the saturation distribution can be computed analytically. For more complex structures, such as geostatistically generated heterogeneity fields a quasi-static displacement site-percolation [38] model will be applied. The weighted arithmetic mean of the saturation distribution gives one point on the macroscopic capillary pressure–saturation–relationship.

We will neglect hysteresis effects for the simple geometries, only the drainage curve is computed in these cases. For a more sophisticated geometry also the main imbibition curve is calculated (see section 4.4).

In all the above mentioned examples gravity effects are neglected for the averaging procedure of the saturation distribution. The influence of gravity effects will be examined exemplarily in section 4.5.

For both the wetting and the nonwetting phase the conductivity–distribution can be computed for the above mentioned saturation distribution and thus relative permeability–saturation distribution. Averaging this distribution leads to a point of the macroscopic relative permeability–saturation relationship. As shown above, if we assume capillary equilibrium we can average the multiphase conductivities with the same techniques known from single-phase flow systems. Again, in the context of this paper, we will use analytical solutions for the simple geometries. For more elaborate geometries the renormalisation method is applied. Of course also other methods can be used, as, for example, described by Wen and Gómez-Hernández [41].

Cycling through this procedure with different capillary pressures as boundary conditions one can determine macroscopic capillary pressure–saturation and
relative permeability–saturation relationships.

Fig. 11. Averaging constitutive relations from the local to the macroscale

Before we go into detail regarding the averaging process of the relative permeabilities in a two–phase system we first offer an introduction to the averaging of conductivities.

This will be done first for single phase flow; the approach will then be extended to two–phase flow.

The effective conductivity tensor of a single phase system should meet the following requirements:

- The tensor should be positive definite, which ensures that a positive hydraulic head gradient always results in a positive flux.
- The tensor should be symmetric, because the application of the tensor is then not restricted to the coordinate system it is computed in.
- The tensor should be independent of the boundary conditions, as this would otherwise again restrict its application.

Because the conductivity is not an additive variable volume averaging cannot be applied. However, it is known, that in a layered medium, the effective conductivity parallel to the layers corresponds to an arithmetic mean while that perpendicular to the layers corresponds to a harmonic mean. This implies a dependence of the conductivity not only on the material properties but also on the boundary conditions. To overcome the dependence on the boundary conditions the flux is included in the averaging procedure. An effective conductivity then ensures a unique flux for a given hydraulic head gradient. For the two–phase–flow problems under consideration, like the infiltration of a DNAPL,
the flux is the variable we are interested in. If, on the other hand, travel times of water pollutants were crucial variables, this averaging approach would not suffice as the displacement velocity rather than integral fluxes would be of interest.

For the computation of the effective conductivity as a function of the flux $q$ Equation (7) has to be solved for $K$.

$$q = \pm \int_{\Gamma} \mathbf{v} \cdot d\Gamma = -L\mathbf{K} \text{grad} h$$

Consequently, the fluxes over the length $L$ of the boundaries $\Gamma$ have to be computed.

To average the conductivities, several approaches are possible. They can be divided into the categories experimental, analytical or numerical. Experimental methods will not be discussed here.

The analytical approaches mainly include two means, the arithmetic and the harmonic mean. These means are applied to the different flow directions in a layered medium [12]. Given that each layer is homogeneous and isotropic, which implies a scalar conductivity, the arithmetic mean is computed as follows:

$$\overline{k_{ari}} = \frac{\sum_i (w_i \cdot k_i)}{\sum_i w_i}, \quad w_i := \frac{V_i}{V}.$$  \hspace{1cm} (8)

If the fluid flows perpendicular to the layers, the harmonic mean is applied:

$$\overline{k_{har}} = \frac{1}{\sum_i (w_i \cdot k_i)}, \quad w_i := \frac{V_i}{V}.$$  \hspace{1cm} (9)

Numerical methods are chosen for the computation of effective conductivities of systems with complex geometries. "Block conductivity" methods solve Equation (7) for the whole domain by computing the flow field numerically. Durlowsky [18] gives a detailed overview of block conductivity methods. The disadvantages of this method are, on the one hand, the long computing times and on the other hand, the one resulting effective conductivity tensor; structures below the computed domain cannot be detected.
Ewing et al. [20] and Arbogast et al. [3] have integrated the computation of the conductivities in the numerical algorithm for the solution of the (multi-phase) flow equations. The combination with efficient solvers such as multigrid techniques leads to fast algorithms. However, a physical interpretation of the values, as is desirable here, is no longer possible.

Renormalisation methods are a compromise between numerical efficiency and physically interpretable results. They treat easy-to-handle subdomains of the domain. For a quadratic domain (see Figure 10), the effective horizontal conductivity $k_h$ can be computed with a finite difference method [28, 42]:

$$k_h = \frac{2 \cdot (k_1 + k_2) \cdot (k_3 + k_4) \cdot (k_{12}^h + k_{34}^h)}{3 \cdot (k_1 + k_3) \cdot (k_2 + k_4) + \frac{1}{2} \cdot (k_1 + k_2 + k_3 + k_4) \cdot (k_{12}^h + k_{34}^h)},$$

with $k_{ij}^h = \frac{2 \cdot k_i \cdot k_j}{k_i + k_j}$.

(10)

For the effective vertical conductivity, only the indices "2" and "3" have to be exchanged. After having found the average for the four cells, one goes to a higher scale and again averages (averaged) four cells (see Figure 10). Thus the averaging is conducted on different hierarchies. Larger systems can be subdivided into any desired number of quadratic volumes as long as they are divisible by four.
4 Derivation of Constitutive Relationships for Two Phase Flow in a Perfectly Layered Medium applying the Upscaling Toolbox

In the following, the upscaling approach will be applied to a perfectly layered medium. This can be conceptualized as a simple description of a heterogeneous aquifer. The utilisation of such a medium has two advantages. The derived parameters are valid infinitely parallel to the layers and the main axis of the permeability tensor coincides with the main axis of the system. For other media, the coordinate system might have to be transformed.

In a perfectly layered medium the layers and their properties such as porosity or the constitutive relationships alternate periodically with a length of period \( a \) (see Figure 13). The single layers are assumed to be isotropic and homogeneous.

![Perfectly layered medium](image)

Fig. 13. Perfectly layered medium

In our case, one period of the horizontally layered medium contains a 14 cm thick layer of coarse sand (index \( c \)) and a 2 cm thick layer of fine sand (index \( f \)). The material properties of the two sands can be taken from Table 4. For the description of the capillary pressure–saturation–relationship, the parametrisation after Brooks & Corey is applied. Because \( \lambda, S_{wr}, S_{nr} \) do not differ, the relative permeability–saturation–relationship is the same for both sands. This system will subsequently be named the reference case.

<table>
<thead>
<tr>
<th>Material properties for the coarse and the fine sand</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k_0 ) [m(^2)]</td>
</tr>
<tr>
<td>coarse sand</td>
</tr>
<tr>
<td>fine sand</td>
</tr>
</tbody>
</table>
4.1 REV for Two Phase Flow in a Periodically Layered Medium

Before we derive any physical parameters, the size of an REV for effective conductivities in a periodically layered medium with two-phase flow is examined using well known formulas of arithmetic and harmonic averaging (see Equations (8), (9) and Cardwell and Parsons [12]).

Starting from an (arbitrary) point within the domain the size of the averaging volume is successively increased by the thickness of the coarse sand layer. As a criterion for arriving at an REV a deviation of $\epsilon = \pm 5\%$ from the asymptotic solution was chosen.

Fig. 14. Size of REV as a function of the relation of the conductivities of the two layers ($rc = k_{\text{fine}}/k_{\text{coarse}}$)

In a periodically layered medium with two-phase flow, the relation $rc$ of the effective conductivity of the fine sand ($k_{\text{fine}}$) to the effective conductivity parallel to the layers ($k_{\text{coarse}}$) has a distinct influence on the size of the REV. As a result of the varying saturations, the relation $rc$ of the effective conductivities varies between $10^{-3}$ and $10^{3}$ (see Figure 14). For a relation of the conductivities $rc = 1.0$, the medium can be considered homogeneous and isotropic. The size of the REV is thus not of importance. A look at the arithmetically weighted values for the flow parallel to the layers shows a symmetric course of the curve. The numbers of periods necessary to derive an REV increases for values smaller and larger than $rc = 1.0$ but always remains smaller than two.

For the harmonically weighted values for the flow direction perpendicular to the layers, the curve is more complicated. For $\sim 0.5 \cdot 10^{-1} < rc < 1$, the size of the REV is larger than in the arithmetically weighted case, arriving at a
maximum value of four periods at \( rc > \sim 10^{-1} \). For values of \( rc \) smaller than that the size of an REV decreases again as the effective conductivity of the less permeable layer becomes very small, meaning that the saturation is very low. Consequently, the less permeable layer dominates the system. Thus only small averaging volumes are required to provide an REV. When \( rc \) becomes higher than 1.0, the thickness and thus the influence of the less permeable layers increases. In the case of the harmonic average, less permeable layers are weighted more strongly than the more permeable layers. Consequently, we arrive at an REV after less than 0.5 periods of layers.

Summarising, one can state that at the most four periods of layers are required to derive a REV for effective conductivities in the case of a periodically layered medium with two–phase flow. For averaging values smaller than four periods, a discrepancy might arise between numerical solutions using the effective conductivities and those using the discrete values for the intrinsic and relative permeabilities.

### 4.2 Upscaling of the Capillary Pressure–Saturation – Relationship

Again, we will use the simple case of a layered medium to demonstrate the averaging process for the transition from the local to the macroscale for the capillary pressure–saturation–relationship.

With the assumption of a capillary equilibrium and neglecting gravity effects we compute the macroscopic capillary pressure–saturation–relationship as described at the beginning of this chapter. A striking result of a comparison of the capillary pressure–saturation–relationships of the two sands with the averaged, macroscopic capillary pressure–saturation–relationship (see Figure 15) is that the macroscopic \( P_c - S_w \)–relation equals the \( P_c - S_w \)–relation of the coarse sand especially for high saturations. Moreover in the case of low saturations, the curves do not differ much either. This is due to the higher volume fraction of the coarse sand.

If the averaged macroscopic capillary pressure–saturation–relationship were to be used for a numerical simulation of the infiltration of a DNAPL into a water–saturated domain, the horizontal mobilisation of the DNAPL would not be represented correctly. In such a case, the entry pressure of finer materials delays the vertical spreading of the DNAPL, yet the entry pressure of the fine material is not represented in the macroscopic capillary pressure–saturation–relationship (see also Figure 5 of the motivation example). Consequently, for the upscaling procedure presented here, another averaged parameter must be found which represents the interaction of the layered medium with the two fluids more appropriately. It is worth to point out that even if we figured out
capillary forces to be one of the dominant processes in the upscaling procedure, averaged capillary pressure–saturation–relationships do not explain the macroscopic behaviour of multiphase flow in heterogeneous systems.

4.3 Upscaling of the Relative Permeabilities

Based on the saturation distributions of the wetting and the nonwetting phase and on the Brooks–Corey functions for the relative permeabilities, a distribution of the relative permeabilities can be calculated for the periodically layered medium as depicted in Figure 13. For a perfectly layered medium, the averages can be obtained analytically. Equation (11) defines the relative permeability of the wetting phase in the horizontal direction which is parallel to the layers.

$$
\frac{k_{rwh}(S_w)}{k_h(S_w = 1)} = \frac{b \cdot k_{rwf} \cdot k_t + (1 - b) \cdot k_{rcw} \cdot k_c}{b \cdot k_t + (1 - b) \cdot k_c}
$$

Equation (12) gives the relative permeability for the wetting phase in the vertical direction perpendicular to layers.
where the index \( w \) denotes the wetting phase. The indices \( f, c \) identify the fine and the coarse sand respectively. The equations for the relative permeability for the non-wetting phase can be set up accordingly. The results of the averaging procedure are shown in Figure 16.

![Figure 16](image)

**Fig. 16.** Macroscopic relative permeability–saturation–relationship for layered medium

The averaged relative permeabilities show courses of the curves for the wetting and the nonwetting phase parallel to the layers (horizontal flow) different to those for the phases perpendicular to the layers (vertical flow). Consequently, a macroscopic saturation–dependent anisotropy evolves, depending solely on the heterogeneities on the macroscale. On the local scale, the layers are assumed to be isotropic.

In order to illustrate the saturation dependent macroscopic anisotropy further, the relation of the horizontal conductivity \( (k_h) \) and the vertical conductivity \( (k_v) \) for water and DNAPL \( a = k_v/k_h \) is plotted against the water saturation (see Figure 17).

For a water saturation of \( S_w = 1.0 \), the anisotropy of the conductivity of the water and of the single phase flow case (horizontal line in Figure 17) coincide (Marking 3 in Figure 17). When the water saturation is reduced, the water still occupies the fine sand alone, but retreats from the coarse sand where
the DNAPL starts to infiltrate. Thus, the relative permeability for the water in the coarse sand decreases. At a saturation of $S_w = 0.617$, the conductivity for water in the coarse sand is reduced to 10% of the saturated conductivity. Consequently, the two layers possess the same conductivity for the water phase ($k_v = k_h$) and the relation of the anisotropy becomes $a = 1.0$ (Marking 2 in Figure 17). When the water saturation is reduced further the system becomes less and less permeable for water. Now the the fine sand is more permeable than the coarse sand because at low saturations the water retreats to the finer material. Thus especially in the vertical direction the effective conductivity for water is reduced.

For $S_w < 0.17$, the relative permeability and thus the conductivity approach zero (Marking 1 in Figure 17).

The anisotropy of the DNAPL conductivities does not exceed $a = 0.53$ for a saturation of DNAPL of $S_n = 1.0$ (see Figure 17). In the case of high DNAPL and low water saturations, the water infiltrates into the fine sand first, while the DNAPL still occupies the coarse sand with its higher intrinsic permeability. The relative permeability for the DNAPL phase in the fine sand decreases first, and the relative permeability for the nonwetting phase in the coarse sand decreases as well. As both values decrease the anisotropy remains at values near zero. When the water saturation has reached $S_w = 0.2125$, the water as the wetting phase completely occupies the fine sand. Consequently, the relative permeability for the nonwetting phase in these layers decreases to
zero and the whole medium becomes impermeable for the nonwetting phase in the flow direction perpendicular to the layers. As the conductivity \( k_v \) thus becomes zero, the anisotropy also becomes zero.

On the macroscale, the vertical conductivities of the DNAPL can only exceed zero when the entry pressure of the fine sand has been overcome. This happens at a macroscopic DNAPL saturation of \( S_n = 0.7875 \). This saturation is therefore called the **macroscopic residual saturation of the nonwetting phase**. The corresponding water saturation is called the **macroscopic residual saturation of the wetting phase**. Again, these residual saturations can only be identified on the macroscale whereas there are no residual saturations defined at the same time on the local scale. The size of macroscopic residual saturations depends on the entry pressure of the fine material and the thickness ratio of both layers [9].

The above described upscaling procedure was validated with a numerical experiment using a periodically layered 2D system where DNAPL infiltrated from the top. The results were published in [8].

### 4.4 Hysteresis effects on the Macroscale

With a complex heterogeneity distribution the appearance of hysteresis effects on the macroscale will be shown. With the program r2df [19, 39] a permeability field with the following parameters is generated (see also Figure 18):

- average permeability \( \log(k_{0,\text{ref}}) = -10.34 \),
- standard deviation \( s = 0.4315 \) and
- anisotropy factor \( a = 10 \)

Then the Brooks-Corey parameter \( P_D \), the entry pressure, is scaled with the help of the Leverett function (14).

\[
\begin{align*}
P_c &= \frac{P_D}{\sqrt{S_w}} \quad (13) \\
P_D &= P_{D,\text{ref}} \cdot \sqrt{\frac{k_{0,\text{ref}}}{k_0}} \quad (14)
\end{align*}
\]

As the average or reference entry pressure \( P_{D,\text{ref}} = 550 \text{ Pa} \) is chosen. The Brooks-Corey parameter \( \lambda \) is set constant (\( \lambda = 2.0 \)) throughout the whole domain.

Based on this distribution of different local constitutive relationships a site-percolation model yields saturation distributions for each capillary pressure
Fig. 18. Generated heterogeneity field and its macroscopic $P_c - S_w$ relationship applied at the boundary assuming capillary equilibrium and neglecting gravity forces. The arithmetic mean of the saturation distribution together with the appertaining capillary pressure gives one point of the macroscopic $P_c - S_w$. With a renormalisation method the average conductivities and thereby the relative permeabilities are computed on the basis of the saturation distribution arithmetically in the x–direction and harmonically in the y–direction.

Looking at the imbibition curve of the resulting $P_c - S_w$ relationship (see Figure 18) it is obvious that the nonwetting phase is trapped in the domain at low capillary pressures. This effects a macroscopic residual saturation of the nonwetting phase. The trapping occurs when regions with high permeability and low entry pressure still possess a saturation of the nonwetting phase at low capillary pressures while surrounding regions with lower permeabilities and higher entry pressure are already fully saturated with water and thus do not provide a mobility for the DNAPL to flow out of the high permeability regions.

Fig. 19. Relative Permeability–Saturation relationship for the drainage (left) and the imbibition (right) curve for a geostatistically generated heterogeneity field
The relative permeability-saturation relationship for the drainage and the imbibition cycle both show a saturation dependent anisotropy (see Figure 19). However no pronounced hysteresis effects can be detected. For the nonwetting fluid the relative permeabilities do not show distinct hysteresis because at small capillary pressures the saturation of the phase and thus its relative permeability is low anyway. The nonwetting phase only becomes mobile at saturations higher than $S_n = 0.62$. This threshold value corresponds to a residual saturation. The threshold value depends on various parameters like e.g. the dimension of the percolation model or the kind of spatial discretisation [38].

For the wetting fluid the relative permeabilities of the drainage and imbibition curve show a similar behaviour for saturations of the wetting phase of up to $S_w \simeq 0.9$. Then the residual saturation of the nonwetting phase is reached, meaning the saturation of the wetting phase cannot be increased further. At the residual saturation of the nonwetting phase, the relative permeability of the wetting phase becomes one. Thus, a hysteresis effect on the macroscale arises not only for the $P_c - S_w$ relationship but also for the $k_{rw} - S_w$ relationship.

4.5 Including the Gravity Force in the Averaging Procedure

In order to illustrate the influence of the gravity force on the effective parameters, we will look at the domain with the periodically altering layers (see Figure 13), taking again the parameters for the different materials as shown in Table 4.

At first, only the coarse background material is examined. Both the wetting (water) and the nonwetting (DNAPL) phase are present in this layer and have not yet infiltrated into the fine sand layer below. The capillary pressure and the pressure of the water phase increase linearly with the depth. Inverting the capillary pressure–saturation–relationship produces the saturation distribution. The saturation of the water phase decreases with increasing depth whereas the saturation of the nonwetting phase increases with increasing depth (see Figure 20).

As the constitutive relations for the layers are known, the distribution of the relative permeabilities can be computed directly from the saturation distributions (see Figure 21).

Because the intrinsic permeability of one layer does not alter, the effective conductivity changes with the depth. Thus, a homogeneous medium might be heterogeneous for two-phase flow problems. We now average the relative permeabilities. Following the reasoning of section 4, the conductivities can be averaged arithmetically in the horizontal and harmonically in the vertical direction.
Rather than using integrals to derive averaged parameters (which leads to complicated systems of equations), we will simplify the problem by disregarding the continuous course of the curves of the saturation and the relative permeability. Instead, these variables are assumed to be piecewise constant (see Figure 20). In order to show the general results of such an approach, it suffices to subdivide the coarse background material into two parts (see Figure 20). With this assumption, the average conductivity can be easily derived in the horizontal

$$\bar{k}_h = k \cdot \frac{1}{2} (k_{r1} + k_{r2})$$  (15)
and vertical direction

\[ k_v = k \cdot \frac{2 \cdot k_{r1} \cdot k_{r2}}{k_{r1} + k_{r2}}. \]  

(16)

Averaging relative permeabilities requires average saturations. In order to average the saturations, at first the capillary pressures at the limits of the intervals are determined in accordance with Equation (17)

\[ P_c = \begin{cases} 
0 & \text{for } z \geq z_0 \\
P_D + (z_0 - z) \cdot (\rho_n - \rho_w) & \text{for } 0 \leq z \leq z_0 
\end{cases}, \]

where \( P_D \) is the entry pressure of the layer.

Now the average saturation of the wetting phase can be computed after Equation (18)

\[ \overline{S_w} = \frac{\int_{P_{cl}}^{P_{cu}} S_w dP_c}{P_{cl} - P_{cu}} = \frac{P_{Dc}^2}{P_{cl} \cdot P_{cu}} = \sqrt{S_{wu} \cdot S_{wl}}, \]

(18)

for the case that the form factor \( \lambda = 2.0 \) and the residual saturations on the local scale are zero.

This corresponds to a geometric mean of the saturations of the water phase at the limits of the intervals. The relative permeability of the interval can be computed with its average saturation. Taking different capillary pressures at the lower boundary, one obtains the relative permeability – saturation–relationship, including the gravity force for the coarse medium (see Figure 22).

Whereas the relative permeabilities of the water phase equal each other in the horizontal and vertical directions for saturations of 1 or 0, the relative permeability of the nonwetting phase depends on the direction for low nonwetting phase saturations. In the vertical direction, from \( S_n = 0.35 \), the nonwetting phase is present in the whole column. Before that, zero saturations result in zero relative permeabilities. In the horizontal direction, the arithmetic mean makes relative permeabilities possible at nonwetting phase saturations below \( S_n = 0.35 \).

Consequently, a homogeneous, isotropic medium can possess a heterogeneous distribution of the effective permeabilities induced by a gravitational process.

Finally, the approach is extended to the periodically layered system (see Figure 22).

Making a comparison of these relations to the ones derived without taking the gravity into account (see Figure 16), several features attract attention.
Fig. 22. Relative permeability–saturation–relationship for the coarse sand (left) and the layered medium (right) including gravity forces

The nonwetting phase saturation now only has to reach $S_n = 0.75$ to enable a vertical relative permeability greater than zero whereas, without gravity forces, it has to reach $S_n = 0.8$. In the case including the gravity forces, the saturation of the DNAPL is greater in the lower part of the layers than in the upper part of the layers. Thus, the entry pressure of the fine sand is reached in the lower part of the coarse sand layer although, on average, the saturation of the nonwetting phase would not suffice to overcome the entry pressure of the fine material. This causes a reduction of the residual saturation of the nonwetting phase by 20%. Correspondingly, the course of the curve of the relative permeability of the water phase in the vertical direction can be explained: until the entry pressure of the fine sand layers has been reached, only the water phase is mobile; thus, the macroscopic residual saturation of the water phase is increased from $S_{wr} = 0.2$ to $S_{wr} = 0.25$.

Note that if we include gravity in the upscaling procedure the total length scale of the averaging volume influences the results. If neglecting gravity the length scale does not play any role.

Summarising, the shown differences of the relative permeability–saturation–relationships are not distinct. However, the differences depend on the size of the averaging volume, which is fairly small in the observed case. When the gravity force is taken into account, the size of the averaging volume has a greater impact than in the approach of the capillary equilibrium. In addition, the arrangement of the heterogeneities in relation to the boundary conditions has to be considered. In the following, the influence of gravity forces will again be neglected.
5 Verification and Application Example

The effective parameters derived with our upscaling approach assuming a capillary equilibrium facilitate the simulation of two–phase flow processes on the macroscale.

In addition to that verification, our approach is applied here to an infiltration experiment [2]. The experimental setup is depicted in Figure 23, Table 5 displays the parameters of the sands used.

![Fig. 23. Setup of infiltration experiment: distribution of the lenses ([2])](image)

**Table 5**

<table>
<thead>
<tr>
<th>Parameters of the sands used in the infiltration experiment ([2])</th>
<th>fine sand</th>
<th>medium sand</th>
<th>coarse sand</th>
</tr>
</thead>
<tbody>
<tr>
<td>permeability $k_0$ [m$^2$]</td>
<td>$6.38 \cdot 10^{-11}$</td>
<td>$1.22 \cdot 10^{-10}$</td>
<td>$2.55 \cdot 10^{-10}$</td>
</tr>
<tr>
<td>entry pressure $P_D$ [Pa]</td>
<td>882.9</td>
<td>539.55</td>
<td>353.16</td>
</tr>
<tr>
<td>form factor $\lambda$ [-]</td>
<td>3.0</td>
<td>3.0</td>
<td>3.2</td>
</tr>
<tr>
<td>residual saturation of water $S_{wr}$ [-]</td>
<td>0.06</td>
<td>0.06</td>
<td>0.06</td>
</tr>
<tr>
<td>residual saturation of DNAPL $S_{nr}$ [-]</td>
<td>0.10</td>
<td>0.15</td>
<td>0.10</td>
</tr>
<tr>
<td>porosity $\phi$ [-]</td>
<td>0.38</td>
<td>0.38</td>
<td>0.38</td>
</tr>
<tr>
<td>volume fraction $w_i$ [%]</td>
<td>10</td>
<td>80</td>
<td>10</td>
</tr>
</tbody>
</table>

During the experiment a DNAPL (Trichlorethylene, TCE), with a density of $\rho = 1460$ kg/m$^3$ and a dynamic viscosity of $\mu = 0.57 \cdot 10^{-3}$ kg/m·s infiltrated with a constant flux of $29$ ml/min along a length of $0.02$ m at the top. After 2970 s the influx was stopped.

In order to simulate this experiment numerically, different approaches can be used to derive the required parameters which lead to a varying accuracy.
and which differ in their necessary input. An acceptable upscaling procedure should require as little information about the system as possible and, at the same time, should be as precise as necessary. Here, we compare two different upscaling approaches. First, we apply a simple geometric average of the parameters, taking only the volume fractions of the different sands into account. This is a well known approach in averaging single phase flow parameters [40]. We then average the constitutive relationships for two different geometric arrangements of the sands.

In the first case, it is assumed that all the sands are perfectly mixed. The effective parameters were then derived using a weighted geometric mean according to the volume fractions of the different sands. The resulting constitutive relationships resemble those of the medium sand because it has the highest volume fraction. The relative permeability–saturation–relationship (see Figure 24) is isotropic, because no information about the geometric arrangement of the sands entered the calculation.

These constitutive relationships were applied in a numerical simulation of the experiment described above. Figure 25 shows its result (isolines) compared to the experimental results (hatched areas) after one hour.

Because a Neumann boundary condition is applied in the numerical simulation in accordance with the experimental setup, the infiltrated volumes of DNAPL are the same in the experiment and the simulation. The numerical simulation shows that the averaging approach of the weighted geometric mean does not suffice to reproduce the experimental results correctly. The infiltration of the DNAPL in the vertical direction is overestimated whereas the dispersion in the horizontal direction is underestimated.
Fig. 25. Comparison of the saturation distribution of the DNAPL after one hour: numerical simulation with effective parameters derived by a weighted geometric mean (isolines) and experimental results (hatched areas).

Consequently, in addition to the information about the volume fractions, the geometric arrangement of the materials in the tank is taken into account by applying our upscaling approach.

First constitutive relationships are computed assuming a layered arrangement of the sands. The medium sand is the background material; a layer of the coarse sand is embedded in the upper part and a layer of the fine sand is embedded in the lower part (see Figure 26).

Fig. 26. Geometry of the averaging volume of a layered medium

Figure 27 presents the resulting constitutive relationships. The relative permeability – saturation–relationship now has an anisotropic character.

The anisotropy can be related to characteristic points in the capillary pressure–saturation–relationships of the sands. As long as the capillary pressure is higher than the entry pressure of the coarse sand and lower than the entry pressure of the medium sand, the DNAPL can only infiltrate into the coarse sand. This holds up to an average water saturation of $S_w = 0.802$. The coarse
sand can only be penetrated from the sides; consequently, there is only a horizontal mobilisation. With decreasing water saturation, the capillary pressure increases until the entry pressure of the medium sand has been overcome. The entry pressure of the fine sand is reached at an average water saturation of $S_w = 0.291$. From then on, the DNAPL can also spread in the vertical direction.

Correspondingly, residual saturations of the nonwetting fluid appear in the horizontal and vertical directions. Taken that the fluid is no longer mobile at a saturation lower than $S_n < 1.0 \cdot 10^{-4}$, the residual saturations can be defined. The residual saturation of the nonwetting fluid is much higher in the vertical direction ($S_{nrv} = 0.714$) than in the horizontal direction ($S_{nrh} = 0.145$). These residual saturations have to be exceeded before the nonwetting fluid becomes mobile and spreads in the respective direction.

When the results of the numerical simulation employing the constitutive relationships for the layered medium are compared, (see Figure 28) it is obvious that the spreading of the DNAPL in the horizontal direction is overestimated in the simulation, whereas the mobilisation is not high enough in the vertical direction.

In the last example, the information that the fine and the coarse sand were incorporated as lenses into the sand tank is taken into account. The dimension of the tank (length = 1.20 m, height = 0.50 m), the lenses (length = 0.20 m, height = 0.02 m), and the volume fractions of each sand enter the derivation of an REV (see Figure 29). The postulation that the fine and coarse sand lenses should be in contact is also incorporated. The actual position of the layers in the REV is arbitrary, other arrangements would lead to slightly different
Fig. 28. Comparison of the saturation distribution of the DNAPL after one hour: numerical simulation with effective parameters derived with the upscaling approach for a layered medium (isolines) and experimental results (hatched areas) effective parameters. For instance, embedded lenses would lead to hysteresis effects.

Fig. 29. Geometry of the averaging volume for the application of the upscaling approach to a medium with lenses

The constitutive relationships shown in Figure 30 were computed with the upscaling approach (quasianalytical approach after Kasap and Lake [27]). As the capillary pressure and the saturation are scalar quantities, they are both averaged with an arithmetic mean. Consequently, the geometry has no influence and the capillary pressure–saturation–relationship equals that of the layered medium.

The relative permeability–saturation–relationship shows an anisotropy for both phases; however, this is not as pronounced as in the case of the layered medium. A comparison of the residual saturations (see Table 6) of the layered medium and the medium with lenses shows that the differences in the residual saturations of water are not distinct. As far as the residual saturation of the
Fig. 30. Constitutive relationships for the case of the upscaling approach applied to a medium with lenses, A) relative permeability–saturation–relationship, B) capillary pressure – saturation–relationship

DNAPL is concerned, it differs by only 0.066 in the horizontal direction. In the horizontal direction in both cases, the entry pressure of the coarse sand is mainly responsible for the start of the mobilisation. In the vertical direction, the residual saturation is reduced from \( S_{nr} = 0.714 \) in the layered case to \( S_{nr} = 0.242 \) in the case of the lenses. In the layered medium, the entry pressure of the fine sand has to be reached before the DNAPL can spread in the vertical direction. In the medium with the lenses, the DNAPL can spread in the vertical direction (along the side of the fine sand lense) as soon as the entry pressure of the medium sand has been overcome.

Table 6

<table>
<thead>
<tr>
<th></th>
<th>( S_{wr} )</th>
<th>( S_{nr} )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>horizontal</td>
<td>vertical</td>
</tr>
<tr>
<td>experiment</td>
<td>0.06</td>
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<tr>
<td>isotropic medium, geometric mean</td>
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<td>0.06</td>
</tr>
<tr>
<td>layers, upscaling approach</td>
<td>0.102</td>
<td>0.192</td>
</tr>
<tr>
<td>lenses, upscaling approach</td>
<td>0.116</td>
<td>0.172</td>
</tr>
</tbody>
</table>

The comparison of the numerical simulation with the effective parameters for the REV with the lenses to the experimental results (see Figure 31) shows a good agreement between the simulation and the experiment. The simulation reproduces the spreading in the horizontal direction and, at the same time, does not underestimate the infiltration in the vertical direction as it does with the parameters of the layered medium.
The results of the numerical simulation taking the parameters of the REV with the lenses does not show all the details of the spreading of the DNAPL in the experiment. This cannot be achieved with upscaled parameters. However the isolines encompass the main part of the infiltrated area and do reproduce the characteristics of the mobilisation process.

![Comparison of the saturation distribution of the DNAPL after one hour: numerical simulation with effective parameters derived with the upscaling approach for a medium with lenses (isolines) and experimental results (hatched areas)](image)

**Fig. 31.** Comparison of the saturation distribution of the DNAPL after one hour: numerical simulation with effective parameters derived with the upscaling approach for a medium with lenses (isolines) and experimental results (hatched areas)

### 6 Conclusion

During the upscaling process new effects evolve on the macroscale which do not occur on the local scale. First of all, a saturation–dependent anisotropy of the relative permeability–saturation – relationship can be observed. The two–phase flow behaviour amplifies the anisotropy of the effective conductivity as compared to single phase flow. Furthermore, direction–dependent macroscopic residual saturations evolve where the phases are immobile. Residual saturations are an important parameter for assessing the success of remediation processes, for example. For remediation methods also hysteresis effects are of interest. With a complex heterogeneity field it was shown that hysteresis effects in the capillary pressure–saturation–relationship can be observed on the macroscale though for the local scale no history dependent \( P_c - S_w \) relationships were assumed.

The application of our upscaling procedure proved that the structures of a porous medium on the local scale, such as layers or lenses, have an important influence on the effective parameters on the macroscale. The incorporation of the geometry of these structures in the upscaling process enhances the
quality of the effective parameters on the macroscale and we are thus able, for example, to reproduce the infiltration behaviour of a DNAPL.

Two phase flow parameters can be up-scaled from the local to the macroscale with the presented up-scaling approach. It should be stressed again that this method is restricted to the scale transition from the local to the macro-scale (as discussed in section 1), and cannot be extended to other arbitrary scale transitions. The advantages of this approach are its easy application, e.g. to laboratory experiments, and its physical motivation which allows a physical interpretation of the effective parameters.

When dealing with natural systems one usually has some basic information about the geological structures. Together with the parameters of the different soil or rock types constitutive relationships for the macroscale can be derived with the here presented approach. The thus identified constitutive relationships reproduce the effects of the heterogeneities on the multiphase flow behaviour. Consequently one does not need to discretise the geological structures on the macroscale which accelerates the numerical performance.

The extension of the method to more dimensions, different geometries or more phases can be easily done. However, the assumption of the capillary equilibrium restricts the method so that the weakening of the assumption either for arbitrary boundary conditions or for the inclusion of dynamic effects should be examined in the future.

7 Acknowledgements

We would like to thank Jane Allan [2] for making their experimental data available to us. The work was funded by the Sonderforschungsbereich SFB 404 ’multifield problems in solid and fluid mechanics’ at the University of Stuttgart and the research project ’MUSKAT, multi scale transport’, funded by the German Research Foundation (HE 2531/2-2).

8 Notation

Vectors and matrices are written in bold type.
Averaged values are overlined (e.g. $\bar{k}$).
<table>
<thead>
<tr>
<th>symbol</th>
<th>unit</th>
<th>signification</th>
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</thead>
<tbody>
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<td>$a$</td>
<td>-</td>
<td>anisotropy factor</td>
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<tr>
<td>$A$</td>
<td>$m^2$</td>
<td>area</td>
</tr>
<tr>
<td>$b$</td>
<td>-</td>
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<td>$D$</td>
<td>m</td>
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<td>$m/s^2$</td>
<td>gravitation</td>
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References


