Effective equations for two–phase flow in porous media: the effect of trapping at the micro scale

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Abstract

In this paper we consider a two-phase flow model in a heterogeneous porous column. The medium consists of many homogeneous layers that are perpendicular to the flow direction and have a periodic structure. Trapping may occur at the interface between a coarse and a fine layer. Assuming that capillary effects caused by the surface tension are in balance with the transport, we apply the homogenization approach to derive an effective (upscaled) model. Numerical experiments show a good agreement between the effective solution and the averaged solution taking into account the detailed micro structure.

1 Introduction

Two-phase flow processes in heterogeneous porous media occur in various natural systems. For example, when considering groundwater remediation, or oil recovery from reservoirs. Usually these natural systems display heterogeneities that range from small scale inclusions or lenses to large scale formations. Two different homogeneous materials are often separated by a sharp interface, the transition from one material to another being non–smooth. A significant amount of research has been undertaken to quantify the effects of such transitions on the movement of the phases. One of the first qualitative studies of the effects of heterogeneities on two phase porous media flow has been done by Kueper et al. [12]. Laboratory experiments using a porous column with periodically varying permeability were performed by van Lingen [16].

In the case of small scale heterogeneities, the geological information is hardly ever available. Moreover, even if complete information could be obtained, the computational effort required to perform complete simulations on the small scale is immense. Therefore, it is necessary to obtain effective equations, parameters or constitutive relationships, being able to capture the effects of small scale heterogeneities and transfer them to our modeling scale. There exists a variety of methods to obtain effective or upscaled descriptions. We refer to Wen and Gomez [18] and Darman et al. [4] for overviews.

In this paper we employ homogenization techniques to describe the effect of small scale heterogeneities. The essence of this approach, together with many examples, is explained in [10]. Homogenization techniques have been successfully applied by Neuweiler and Cirpka [17] and Lewandowska et al. [15] to upscale flows in unsaturated porous media. This paper is a continuation of van Duijn et
al. [5], where two phase flow with trapping at the micro scale is considered. In this paper we consider the capillary limit case of [5], in which the capillary effects caused by surface tension are in balance with transport. In the dimensionless setting this is expressed by a capillary number of order one. In the absence of a rigorous mathematical proof for the convergence of the homogenization procedure, the results in [5] are obtained assuming that the first order term in the asymptotic expansion of the oil saturation is continuous across the interfaces separating the homogeneous layers. This leads to enhanced diffusive effects in the resulting effective equation. In this paper we assume the continuity of the first order term in the asymptotic expansion of the capillary pressure, thus giving up the continuity of the corresponding term for the oil saturation. Even though these assumptions refer to terms of small order, they lead to different macro scale results, as we will see below.

In Section 2 we present the model and give the governing equations and interface conditions. Further, the model is transformed into a dimensionless setting in which the capillary number appears. In Section 3 we briefly recall the homogenization approach and derive the effective equations incorporating the small scale interface conditions. The results are discussed in Subsection 3.2. Numerical simulations are performed in Section 4. There we compare the solution of the effective equation to the result of simulations of the fine scale, i.e. multi-layered, flow process. The paper concludes with some final remarks.

2 The model

In this section we describe the specific two phase flow model and the conditions at the interfaces separating two different homogeneous media.

2.1 Model: set–up, equations and assumptions

The medium is assumed to consist of periodically repeating homogeneous layers that are perpendicular to the flow direction. This results in a one-dimensional flow and a spatially periodic medium consisting of alternating coarse and fine layers. For the simplicity of presentation we assume here that the layers have a constant porosity $\Phi$, but a variable absolute permeability $k = k(x)$ that is assumed constant inside each of these layers. Therefore we investigate the one dimensional flow of two immiscible and incompressible phases (water being the wetting phase, oil the non-wetting phase) through a periodic medium with alternating homogeneous high and low permeability zones. The ratio of the (micro scale) homogeneous layer thickness $L_y$ and the (macro scale) column length $L_x$ is assumed small – see Figure 1.

The governing equations are the mass conservation:

$$\phi \frac{\partial S_\alpha}{\partial t} + \frac{\partial q_\alpha}{\partial x} = 0 \quad \text{(with } \alpha = n, nw),$$

(1)
and the extended Darcy law:

\[ q_\alpha = -k(x) \frac{k_{r\alpha}(S_\alpha)}{\mu_\alpha} \frac{\partial p_\alpha}{\partial x}. \]  

(2)

The system is closed with the complementary conditions

\[ S_{nw} + S_w = 1; \]  

(3)

\[ p_{nw} - p_w = p_c(x, S_w). \]  

(4)

Here \( \phi, S, \mu, p, \text{ and } q \) denote the porosity, the saturation - mapped to the standard interval \([0, 1]\), the viscosity, the phase pressure and the specific discharge, respectively, with subscripts for each of the phases. \( k \) denotes the intrinsic (absolute) permeability, and \( k_r \) is the relative permeability of the respective phase.

The capillary pressure is described by the Leverett model [14]

\[ p_c(x, S_w) = \sigma \sqrt{\frac{\phi}{k(x)}} J(S_w). \]  

(5)

where \( \sigma \) and \( J \) are the interfacial tension between the two fluids and the Leverett function, respectively. Here we assume that \( J \) is strictly decreasing, going to infinity as \( S_w \searrow 0 \), and that \( J(1) > 0 \). Physically this means that the pressure difference in the two phases should exceed the capillary entry pressure given by \( p_c(x, 1) = \sigma \sqrt{\frac{\phi}{k(x)}} J(1) \), before the oil can enter into a fully water saturated medium. We immediately see that the entry pressure is inversely proportional to the square root of the permeability, and therefore varies between the layers.

Equations (1) and condition (3) imply that the total specific discharge \( q := q_o + q_w \) is constant in space. Throughout this paper we consider it constant in
time as well. Therefore we assume \( q > 0 \) being a given quantity, meaning that the flow takes place from left to right. Having this in mind we can combine equations (1), (2) and conditions (3), (4) into a single transport equation for the oil saturation,

\[
\frac{\partial S_{nw}}{\partial t} + \frac{\partial}{\partial x} \left[ \frac{k_{nw} - k(x)}{k_{nw} + k_w \mu_o/\mu_w} q - \frac{k_{nw} k_w}{k_{nw} + k_w \mu_o/\mu_w} \frac{\partial p_c}{\partial x} \right] = 0
\]

(6)

For being consistent with [5], we set

\[
u = S_{nw} \quad (S_w = 1 - u)
\]

(7)

and redefine \( k_{rw}, p_c \) and \( J \) in terms of \( u \). In this way \( J \) becomes strictly increasing in \( u \), goes to infinity as \( u \to 1 \) and \( J(0) > 0 \).

With \( L_x \) being a characteristic macroscopic length scale and \( K \) a characteristic permeability, we apply the scalings

\[
\hat{x} := \frac{x}{L_x}, \quad \hat{t} := \frac{t q}{\phi L_x}, \quad \hat{k} := \frac{k}{K},
\]

(8)

the hats indicating dimensionless variables. However, in what follows we give up the hats, all the variables and unknowns having no dimensions. We do this to simplify the notation. In this way we bring (6) to a dimensionless form

\[
\frac{\partial u}{\partial \hat{t}} + \frac{\partial F}{\partial \hat{x}} = 0,
\]

(9)

with

\[
F = f(u) - N_c k(x) k_{rw}(u) f(u) \frac{\partial}{\partial x} p_c(x, u).
\]

(10)

Here

\[
f(u) = \frac{k_{rw}(u)}{k_{ro}(u) + M k_{rw}(u)}
\]

(11)

is the fractional flow function, and

\[
p_c(x, u) = \frac{J(u)}{\sqrt{k(x)}}
\]

(12)

is the capillary pressure. The capillary number \( N_c \) and the viscosity ratio \( M \) from above are defined as follows

\[
N_c = \frac{\sigma \sqrt{K \phi}}{\mu_o L_x}, \quad M = \frac{\mu_o}{\mu_w}.
\]

(13)

Depending on the specific application, the value of the capillary number \( N_c \) may vary considerably. In [5], the consequences of having a moderate and a small value for \( N_c \) are analyzed separately, resulting into different types of effective equations. Here we concentrate on the case of moderate \( N_c \).
2.2 The entry pressure effect

Physical experiments [11, 12] have shown that the capillary forces have an important influence on the two-phase flow behavior in porous media. This impact is easy to recognize in heterogeneous soils, especially at the interfaces between different materials. The so-called entry pressure effect, i.e. the inability of a non-wetting fluid to invade a fine grained material, has been observed in the aforementioned experiments and was thereafter also discussed and modeled in a couple of papers [9, 13].

The entry pressure effect can be modeled explicitly in the Brooks-Corey [3] setting. Referring to (5) and since we have written everything in terms of the oil saturation \( u = S_o = 1 - S_w \), the entry pressure is defined by

\[
p_e(x, 0) = \sigma \sqrt{\frac{\phi}{k(x)}} J(0).
\] (14)

Here and below the dimensionless absolute permeabilities of the coarse and the fine medium are denoted \( k^+ \) and \( k^- \), respectively. Then \( k(x) = k^+ \) if \( x \) is located in a coarse layer and \( k(x) = k^- \) for \( x \) inside a fine-layer. Since \( k \) is different inside two adjacent homogeneous layers, the entry pressure will be discontinuous at the interface separating the two layers. The situation is different, for example, in the parameterization proposed by van Genuchten [8]. There \( p_e(x, 0) = 0 \), so the entry pressure effect is not present anymore.

In the current setting, due to the non-zero entry pressure, the capillary pressure can only be continuous if both phases are present on each side of the interface. Then both phase pressures are continuous, too. On the other hand, if oil is absent in the fine material, the difference in the entry pressure leads to a discontinuous capillary pressure. Recalling (12), this can be expressed in terms of a threshold saturation (entry point), which has to be exceeded before the non-wetting phase can enter the fine layer. This threshold saturation \( u^* \) is uniquely defined by

\[
\frac{J(u^*)}{\sqrt{k^+}} = \frac{J(0)}{\sqrt{k^-}}.
\] (15)

The above discussion is presented in Figure 2. One can easily see there that the continuity in the capillary pressure can only be achieved if the oil pressure \( u \) in the coarse layer exceeds the entry point \( u^* \).

If the above situation is encountered in a one-dimensional setting, it leads to the so-called trapping effect: the oil flow is blocked at the interface between a coarse and a fine material. This blocking is encountered as long as the oil saturation at the coarse side of the interface does not exceed the entry point. In the water-driven oil recovery, this means that a certain amount of oil will be trapped at such interfaces. The maximal amount of trapped oil depends on the
properties of the layered reservoir and can be determined effectively (see [2], [5] and [7] for details).

In a two- or three-dimensional setting, the entry pressure effect causes a lateral spreading and an eventual bypassing of the less permeable obstacle, since the non-wetting fluid will invade the more permeable media first.

Due to the possible discontinuity in the capillary pressure, it is difficult to interpret the equations (9) and (10) across interfaces, where $k$ is discontinuous. To overcome this inconvenience, van Duijn et al. [7] have proposed to consider equation (9) only in the homogeneous layers (where $k$ is constant), and to impose matching conditions across $k$-discontinuities. To be specific, we assume that the interface is located at $x = x_i$, and that the highly permeable medium $k^+$ is located on the left of the interface ($x < x_i$). Similarly, the fine material $k^- (k^+ > k^-)$ is located on the right of the interface ($x > x_i$). We denote $u(x_i-, t)$ and $u(x_i+, t)$ the values approached by the saturation $u$ at the time $t$ and as coming from the left side and right side of the interface (with the same interpretation for other quantities), respectively. Further, by

$$[p_e(t)]_{x_i} = p_e(x_i+, t) - p_e(x_i-, t)$$

we mean the jump in the pressure at the interface $x_i$ and at the time $t$. Then, for all $t > 0$, the flux continuity is assumed at $x_i$:

$$F(x_i-, t) = F(x_i-, t).$$

This natural condition is endowed by extended pressure conditions:

$$u(x_i+, t)[p_e(t)]_{x_i} = 0, \quad \text{and} \quad [p_e(t)]_{x_i} \geq 0.$$

Figure 2: Entry pressure condition and corresponding saturation $u^*$
As follows from the above equality, if oil is present on both sides of the interface \((u(x_i+, t) > 0)\), the capillary pressure must be continuous \(([p_c(t)]_{x_i} = 0)\). On the other hand, if the capillary pressure is discontinuous across the interface \(([p_c(t)]_{x_i} \neq 0)\), there is no oil on the fine material side of the interface \((u(x_i+, t) = 0)\). Moreover, the capillary pressure has then a positive jump \(([p_c(t)]_{x_i} \geq 0)\), since on the coarse material side it stays below the entry point. With reference to Figure 2, the pressure condition (17) can be formulated as

\[
\begin{cases}
  u(x_i-, t) < u^* \implies u(x_i+, t) = 0 \\
  u(x_i-, t) \geq u^* \implies \frac{J(u(x_i-, t))}{\sqrt{k^+}} = \frac{J(u(x_i+, t))}{\sqrt{k^-}},
\end{cases}
\]

with \(u^*\) being the entry point defined in (15).

For a simplified setting, a rigorous mathematical justification of the above procedure has been given by Bertsch et al. [2].

### 2.3 Scale effects

The entry pressure effect described in the previous subsection is one of the important features that need to be accounted for in the upscaling procedure. It occurs at each of the interfaces separating two homogeneous layers having different absolute permeabilities. In mathematical terms, this translates into the matching conditions (16) and (18), which have to be fulfilled at the micro scale across any interface.

Our aim here is a rational derivation of an effective equation describing the two-phase flow at the macro scale. To do so, in Section 3 we employ homogenization techniques. The resulting model will include the micro scale entry pressure effect. In particular, as mentioned in Subsection 2.2, local trapping effects can occur due to the interface conditions. Specifically, the non-wetting phase (oil) cannot enter a less permeable (fine) zone until a certain threshold saturation at the interface is exceeded. This leads to a maximal amount of oil that can be trapped inside a coarse layer. Further, once the maximal amount of trapped oil is exceeded in the coarse material, the amount of oil will not sink below that value, unless other kinds of phenomena occur: obstacle bypassing in the multi-dimensional case, or dissolution and degradation effects. Here we disregard these cases.

On the macro scale, the local trapping phenomena lead to a macroscopic residual saturation. This trapped mass of non-wetting phase becomes immobile and cannot be removed by the flow processes. These assertions are sustained by the analysis carried out in Section 3.
3 The homogenized model

In this section we proceed with the derivation of the effective two-phase flow equations. The micro scale trapping effects that are due to the differences in the entry pressure corresponding to different homogeneous layers are also included.

3.1 The homogenization procedure

To end up with an effective model we apply homogenization techniques [10]. We refer to the setting of Subsection 2.1. The heterogeneity enters into the system only through the alternating high ($k^+$) and low ($k^-$) absolute permeabilities, which are repeating as indicated in Figure 3. Each homogeneous layer has a constant thickness $L_y$ (the micro scale reference length), which is much smaller than the macro scale reference length $L_x$. This leads naturally to a small expansion parameter $\varepsilon = L_y/L_x$. Trapping occurs at all transitions from a coarse to a fine layer, as mentioned in Subsection 2.2.

![Figure 3: Permeability distribution on the small scale](image)

A similar approach can be applied to derive effective equations for a different distribution of the homogeneous layers (see van Duijn et al. [5]). This includes micro structures that are randomly distributed with respect to both the location of the permeability jumps and the value of the permeability.

In the simplified (i.e. periodically repeating homogeneous layers of thickness $L_y$) we can assume without loss of generality that the traps are located at the points \{x_i = i\varepsilon\}, i being any integer such that $x_i$ falls inside the domain of our interest. Then the permeability $k := k^\varepsilon(x)$ is defined as

$$k^\varepsilon(x) = \begin{cases} 
  k^+, & \text{if } (2i-1)\varepsilon < x < (2i)\varepsilon, \\
  k^-, & \text{if } (2i)\varepsilon < x < (2i+1)\varepsilon.
\end{cases} \quad (19)$$

We can replace now $k^\varepsilon$ in the dimensionless oil flow equation (9). As mentioned before, this equation holds only in the interior of any homogeneous layer, and the matching conditions defined in (16) and (18) are imposed at the interfaces. The first condition needs no further discussion. Depending on the type of transition
(coarse to fine layer, and vice versa), the pressure condition (18) reads:

\[
\begin{align*}
\text{if } u(2i\varepsilon - 0) < u^*, \text{ then } u(2i\varepsilon + 0) &= 0; \\
\text{if } u(2i\varepsilon - 0) \geq u^*, \text{ then } \frac{J(u(2i\varepsilon - 0))}{\sqrt{k^+}} &= \frac{J(u(2i\varepsilon + 0))}{\sqrt{k^-}},
\end{align*}
\]

(20)

for interfaces located at \(x_{2i} = (2i)\varepsilon\), or

\[
\begin{align*}
\text{if } u((2i + 1)\varepsilon + 0) \geq u^*, \text{ then } \frac{J(u((2i + 1)\varepsilon + 0))}{\sqrt{k^+}} &= \frac{J(u((2i + 1)\varepsilon - 0))}{\sqrt{k^-}}, \\
\text{if } u((2i + 1)\varepsilon + 0) < u^*, \text{ then } u((2i + 1)\varepsilon - 0) &= 0,
\end{align*}
\]

(21)

if the interface is situated at \(x_{2i+1} = (2i + 1)\varepsilon\).

Having in mind the above, we are performing a formal asymptotic expansion with respect to \(\varepsilon\)

\[
u_\varepsilon(x, t) = u^0(x, y, t) + \varepsilon u^1(x, y, t) + \varepsilon^2 u^2(x, y, t) + \ldots,
\]

(22)

where \(y = \frac{x}{\varepsilon}\) is the fast scale, which we introduce here to capture the highly oscillatory processes at the micro scale. The space derivative is then expanded according to

\[
\partial = \partial_x + \frac{1}{\varepsilon} \partial_y.
\]

(23)

A similar expansion can be applied for the flux, the capillary pressure, or the fractional flow.

At this point we should recall the presence of the two dimensionless numbers, \(M\) and \(N_c\). In \([5]\) the viscosity ratio is assumed of order 1, and the cases of moderate and small capillary number \(N_c\) are treated separately. While the results obtained there for the balance case \((N_c = O(\varepsilon))\) were confirmed numerically by a clear convergence of the averaged solution of the full (micro scale) problem towards the effective solution, in the capillary limit case \((N_c = O(1))\) this numerical evidence was difficult to achieve unless diffusion is becoming dominant. This drawback is caused by a micro scale assumption concerning the continuity of the \(O(\varepsilon)\) term in the asymptotic expansion of the oil saturation. In the present work we focus on the capillary limit case and derive a macro scale equation that is suitable also for the flow regimes where the diffusion is not dominating. Here we make a different micro scale assumption: the continuity of the \(O(\varepsilon)\) term in the expansion of the capillary pressure. In neither case have we a rigorous mathematical proof for convergence, therefore we restrict ourselves to compare the numerical results. As revealed by the experiments in Section 4, which are performed for a moderate diffusion, the present approach yields an effective solution that agrees well with the averaged solution of the micro scale model.
Now we can proceed with the derivation of the effective (upscaled, or averaged) equations for the limit \( \varepsilon \downarrow 0 \). With the derivative defined in (23), applying the expansion (22) to (10) and (9), we can equate the terms of different order in \( \varepsilon \) and obtain the following equations:

\[
\varepsilon^{-2} : 0 = \frac{\partial F^0}{\partial y} = \frac{\partial}{\partial y} \left\{ -N_c \sqrt{k(x)} D(u^0) \frac{\partial u^0}{\partial y} \right\},
\]

\[
\varepsilon^{-1} : 0 = \frac{\partial F^0_x}{\partial x} + \frac{\partial F^1_y}{\partial y} = \frac{\partial}{\partial x} \left\{ -N_c \sqrt{k(x)} D(u^0) \frac{\partial u^0}{\partial y} \right\}
\]

\[
+ \frac{\partial}{\partial y} \left\{ f(u_o) - N_c \sqrt{k(x)} \left[ D(u^0) \left( \frac{\partial u^0}{\partial x} + \frac{\partial u^1}{\partial y} \right) + D'(u^0) u_1 \frac{\partial u^0}{\partial y} \right] \right\},
\]

\[
\varepsilon^0 : 0 = \frac{\partial u^0_t}{\partial t} + \frac{\partial F^1_x}{\partial x} + \frac{\partial F^2_y}{\partial y}.
\]

The above equations hold for any \( x \) and \( t \), whereas \( y \) takes values either in \((-1, 0)\), or \((0, 1)\). The diffusivity is defined as

\[
D(u) = k_{rw}(u) f(u) J'(u).
\]

At the interface located in \( y = 0 \), as well as for \( y \) approaching \( \pm 1 \), the fluxes \( F^0, F^1 \) and \( F^2 \) are continuous. Moreover, the extended pressure condition defined in (20) is imposed at \( y = 0 \), whereas (21) is assumed to hold in a periodic sense at the end points of the cell. As shown by van Duijn et al. [5], these conditions can be fulfilled by a solution \( u^0 \) of (24) only if \( F^0 = 0 \), implying that \( u^0 \) does not depend on \( y \) in any of the homogeneous layers. To be specific, with \( c \) and \( \bar{c} \) related by

\[
\frac{J(c)}{\sqrt{k^+}} = \frac{J(\bar{c})}{\sqrt{k^-}}
\]

whenever \( \bar{c} > 0 \), we have

\[
u^0(y) = \begin{cases} c > u^* & \text{for } -1 < y < 0, \\ \bar{c} & \text{for } 0 < y < 1, \end{cases}
\]

if \( c \) exceeds the threshold saturation \( u^* \) and the NAPL can therefore infiltrate into the fine material, or

\[
u^0(y) = \begin{cases} c \leq u^* & \text{for } -1 < y < 0, \\ 0 & \text{for } 0 < y < 1, \end{cases}
\]

if there is no NAPL flow from the coarse into the fine material. In the first case, the capillary pressure is continuous at the interface. Since \( F^0 = 0 \), from (25) we immediately see that \( F^1 \) does not depend on \( y \). Notice that \( F^1 = 0 \) if \( \bar{c} = 0 \).

Due to the complexity of the fine scale problems, which are nonlinear, possibly degenerate, and endowed with complicated boundary conditions, no rigorous
convergence proof has been obtained yet for the homogenization procedure mentioned above. For continuing with the determination of the effective model in the nontrivial case $c > 0$, van Duijn et al. [5] are assuming that $u_1$, the $O(\varepsilon)$ term in the expansion (22) of the saturation, is continuous. Here we propose a different approach: continuity is assumed for $p_c^1$, the first order term in the expansion of the capillary pressure. Even though both assumptions are made on a $O(\varepsilon)$ scale, the resulting macro scale models are different.

To proceed with the derivation of the upscaled model, we first notice that the capillary pressure can be expanded asymptotically as

$$p_c(u_\varepsilon) = \frac{J(u_\varepsilon)}{\sqrt{K}}$$
$$= \frac{1}{\sqrt{K}} \left( J(u^0) + \frac{\partial J(u)}{\partial u} \bigg|_{u^0} \Delta u + \frac{\partial^2 J(u)}{(\partial u)^2} \bigg|_{u^0} (\Delta u)^2 + \ldots \right)$$

with $\Delta u = \varepsilon u^1 + \varepsilon^2 u^2 + \ldots$. (31)

This gives

$$p_c(u_\varepsilon) = \frac{1}{\sqrt{K}} (J(u^0) + \varepsilon u^1 J'(u^0) + \ldots),$$

the dots standing for terms of order $\varepsilon^2$. The first two terms in the $p_c$-expansion are:

$$p_c^0 = \frac{J(u^0)}{\sqrt{K}}$$

$$p_c^1 = \frac{u^1 J'(u^0)}{\sqrt{K}}.$$ (34)

Assuming that $p_c^1$ is continuous in $y = 0$ and at the end points $y = \pm 1$, the interface conditions for $u^1$ become

$$u^1(0-) \frac{J'(c)}{\sqrt{K}^+} = u^1(0+) \frac{J'(c)}{\sqrt{K}^-},$$

$$u^1(-1+) \frac{J'(c)}{\sqrt{K}^+} = u^1(1-) \frac{J'(c)}{\sqrt{K}^-}.$$ (36)

Because $u^0$ is $y$-independent, $F^1$ can be written as

$$F^1 = f(u^0) - N_c \sqrt{K} \left\{ D(u^0) \left( \frac{\partial u^1}{\partial y} + \frac{\partial u^0}{\partial x} \right) \right\}.$$ (37)

Since $F^1$ does not depend on $y$, we can integrate the above on each layer and
end up with

\[ u^1(0-) - u^1(-1+) = \frac{f(c) - F^1}{\sqrt{k^+ N_c D(c)}} - \frac{\partial c}{\partial x}, \quad (38) \]

\[ u^1(1-) - u^1(0+) = \frac{f(\bar{c}) - F^1}{\sqrt{k^- N_c D(\bar{c})}} - \frac{\partial \bar{c}}{\partial x}. \quad (39) \]

Now we can multiply (38) by \( \frac{J'(c)}{\sqrt{k^+}} \), and (39) by \( \frac{J'(\bar{c})}{\sqrt{k^-}} \), and sum up the resulting relations. Using the matching conditions (35) and (36), on the right side all terms cancel out. We therefore are left with

\[ 0 = \frac{J'(c)[f(c) - F^1]}{k^+ N_c D(c)} - \frac{J'(c)\partial c}{\sqrt{k^+}\partial x} + \frac{J'(\bar{c})[f(\bar{c}) - F^1]}{k^- N_c D(\bar{c})} - \frac{J'(c)\partial \bar{c}}{\sqrt{k^-}\partial x}. \quad (40) \]

from which we can determine \( F^1 \) as

\[ F^1 = \frac{J'(c)f(c) + J'(\bar{c})f(\bar{c})}{k^+ D(c) + k^- D(\bar{c})} - N_c \left( \frac{1}{\sqrt{k^+}} \frac{\partial J(c)}{\partial x} + \frac{1}{\sqrt{k^-}} \frac{\partial J(\bar{c})}{\partial x} \right). \quad (41) \]

Using the definition of \( f \) and \( D \) in (11) and (27), with

\[ \lambda(u) = k_w(u)f(u) \quad (42) \]

\( F^1 \) can be rewritten as

\[ F^1 = \frac{1}{k^+ k_w(c)} + \frac{1}{k^- k_w(\bar{c})} - N_c \left( \frac{1}{\sqrt{k^+}} \frac{\partial J(c)}{\partial x} + \frac{1}{\sqrt{k^-}} \frac{\partial J(\bar{c})}{\partial x} \right). \quad (43) \]

It is worth noticing that (43) is derived under the assumption \( \bar{c} > 0 \), meaning also that \( c > u^* \). Whenever \( \bar{c} = 0 \), we have \( F^1 = 0 \) since there is no oil flow.

### 3.2 The effective equation

The effective equation is obtained by integrating (26) in \( y \) over the micro scale cell. For \( F^1 \) we use the expression (43). The last term on the left in (26) disappears, as \( F^2 \) is continuous and periodic in \( y \). With

\[ U(x, t) = \frac{1}{2} \int_{-1}^{1} u^0(x, y, t)dy = \frac{1}{2}(c + \bar{c}). \quad (44) \]

this gives

\[ \partial_t U + \partial_x [\mathcal{F}(U) - N_c A(U)\partial_x \mathcal{P}_C(U)] = 0. \quad (45) \]
The effective saturation is expressed in terms of \( c \) and \( \bar{c} \). For \( \bar{c} > 0 \), using (28) we end up with
\[
\bar{c} = J^{-1} \left( \sqrt{\frac{k^-}{k^+}} J(c) \right).
\]
This gives
\[
U = G(c) := \frac{1}{2} \left( c + J^{-1} \left( \sqrt{\frac{k^-}{k^+}} J(c) \right) \right).
\]
Notice that \( G \) defined above maps \((0, 1)\) onto \((\frac{1}{2}u^*, 1)\). Since \( J \) is strictly increasing, the function \( G \) shares the same property and can therefore be inverted. So we can write \( c \) in terms of \( U \)
\[
c = G^{-1}(U).
\]
Inserting the above into (46) we obtain an equivalent expression for \( \bar{c} \).

With the above expressions we can identify the upscaled fractional flow:
\[
\mathcal{F}(U) = \begin{cases} 
0 & \text{for } 0 \leq U \leq \frac{1}{2}u^*, \\
\frac{1}{k^+ k_u(c)} + \frac{1}{k^- k_u(\bar{c})} & \text{for } \frac{1}{2}u^* < U < 1, \\
\frac{k^+ k_u(c) f(c)}{k^- k_u(\bar{c}) f(\bar{c})} & \text{for } U = 1.
\end{cases}
\]
This function can be interpreted as the weighted harmonic mean of the micro scale fractional flow. The weights, \( 1/(k^+ k_u(c)) \) and \( 1/(k^- k_u(\bar{c})) \), are depending on the relative water permeabilities, which, in turn are depending on \( c \) and \( \bar{c} \).

The upscaled \( A \) term is the harmonic average of the terms \( k^+ \lambda(c) \) and \( k^- \lambda(\bar{c}) \),
\[
A(U) = \begin{cases} 
0 & \text{for } 0 \leq U \leq \frac{1}{2}u^*, \\
2 & \text{for } \frac{1}{2}u^* < U < 1, \\
\frac{1}{k^+ \lambda(c)} + \frac{1}{k^- \lambda(\bar{c})} & \text{for } U = 1.
\end{cases}
\]
To express the upscaled capillary pressure we recall (28). This means that, whenever oil is present on both sides of the interface, the first term in the expansion (32) is constant in the entire micro scale cell. Therefore we get
\[
\mathcal{P}_c(U) = J(c) \sqrt{\frac{k^-}{k^+}} = J(\bar{c}) \sqrt{\frac{k^-}{k^+}}.
\]
To determine the effective diffusivity \( \mathcal{D} \) we use (48), (50) and (51), yielding

\[
\mathcal{D}(U) = \Lambda(U) \mathcal{P}_c(U), \quad \text{where} \quad \mathcal{P}_c(U) = \frac{1}{\sqrt{k^+}} \frac{J'(G^{-1}(U))}{G'(G^{-1}(U))}. \tag{52}
\]

**Remark.** In [5] the effective equation was derived assuming the continuity of \( u^1 \) across the interfaces separating the fine and coarse layers. This yields discontinuities of order \( \varepsilon \) in the capillary pressure. Though small, these discontinuities result in a noticeable effect at the macro scale. In fact, this observation motivated us to write this paper. Without a rigorous mathematical convergence proof one relies on numerical simulations to justify the underlying assumptions. As shown in Section 4, the assumption of continuity of \( p^1_c \) yields better results.

In [5] the first nonzero term in the expansion of the flux reads

\[
F^1 = \frac{f(C)}{\sqrt{k^+} D(C)} + \frac{f(\overline{C})}{\sqrt{k^-} D(\overline{C})} - N_c \left( \frac{\partial C}{\partial x} + \frac{\partial \overline{C}}{\partial x} \right). \tag{53}
\]

By the procedure described above we end up with an effective equation that is similar to (45). In both approaches, the effective functions vanish for \( 0 \leq U \leq 1/2 u^* \), yielding the same maximal amount of trapped oil. The differences occur in the nontrivial case, when \( 1/2 u^* < U < 1 \). In both upscaled equations, the effective fractional flow is a weighted harmonic mean of the micro scale fractional flow. The difference is in the form of the weights. A straightforward calculation shows that the weights in (53) are \( 1/(\sqrt{k^+} k_w(c) J'(c)) \) and \( 1/(\sqrt{k^-} k_w(c) J'(c)) \). These are different from the ones appearing in (49). Further, assuming \( u^1 \) continuous gives directly an effective diffusivity, which is the harmonic mean of the micro scale diffusivities. In (45) we first determine the effective \( \Lambda \) function and next \( \mathcal{D} \) according to (52). The differences are illustrated in the next section for the example considered there, see Figure 4.

### 4 Comparison of upscaled and fine-scale model

In this section we compare the fine-scale numerical simulations with our upscaled model equations. For this we use the numerical simulator MUFTE-UG [1] with a control volume finite element implicit scheme to solve the fine-scale two-phase flow equations and a first order explicit discretization scheme with upwind finite volumes for the upscaled one-dimensional model.

The one dimensional code solves directly the saturation equation (45). For the fine scale simulation performed in MUFTE-UG we use a saturation–pressure formulation for which appropriate initial and boundary conditions have to be added. To be specific, initially the whole domain is in both cases fully oil saturated \( (u = 1) \). For the effective equation we set \( u = 0 \) and \( u = 1 \) at
the left and the right boundary, respectively. The same is considered for the
saturation equation at the micro scale. In addition, the boundary conditions
for the pressure equation are chosen such that the total flux remains constant.

In our example we assume equal viscosities for both phases \((M = 1)\). The two
permeabilities are \(k^- = 0.5\) and \(k^+ = 1\). The capillary number \(N_c\) is set to 1.
The dimensionless interval of computation is \((0, 2)\), yielding \(L_x = 2\). We use
Brooks-Corey type relative permeabilities and Leverett type capillary pressure:
\[
\begin{align*}
 k_{rw}(u) &= (1 - u)^2, \\
 k_{ro}(u) &= u^2, \\
 J(u) &= (1 - u)^{-0.5}.
\end{align*}
\]

This gives an entry point \(u^* = 0.5\), and therefore \(U^* = 0.25\). In this case
the diffusion is not dominating, and the effective model obtained assuming \(u^1\)
continuous was not in good agreement with the averaged fine scale solution. (see
[6]). The effective fractional flows and diffusivities, as computed in this setting
for both the approach in [5] and the present one, are compared in Figure 4.
Notice the enhanced diffusive effects in the former case. One can clearly see that
in both cases the phases are immobile until the upscaled threshold saturation \(U^*\)
has been exceeded. The corresponding effective solutions, computed at \(t = 0.5,\)

![Figure 4](image)

Figure 4: Effective fractional flows (left) and diffusivities (right) obtained for
the present approach (solid) and the approach in [5] (dashed).

are compared in Figure 5. Obviously, the two solutions are not identical. The
solution profile is steeper in the present approach, which is a direct consequence
of the difference in the effective diffusion.

Having in mind the above, it is natural to ask ourselves which of the two effective
models is appropriate. In the absence of a rigorous mathematical proof, our
choice is dictated by the numerical evidence. To this aim we solve the full
problem at the micro scale, with the fine scale domain \((0, 2)\) consisting of \(N\)
cells comprising a coarse and a fine layer. Computations are performed for
\(N\) being 20, 40, or 80. This gives \(\varepsilon = 1/20, 1/40,\) or \(1/80\), and \(L_y = \varepsilon L_x/2\).
For comparison with the effective solution, the computed fine scale solution is
averaged over each micro scale cell. As \(\varepsilon \searrow 0\), the averaged solution converges
towards the effective one. The numerical evidence for convergence is given in Figure 6. The differences on the left side are explained by the fact that the first average point is located further into the domain, this effect being more obvious for larger values of $\varepsilon$. In the flat region, the curves for all values of $\varepsilon$ are on top of each other. A good agreement for the front is achieved only for $\varepsilon = 1/80$.

Figure 7 shows the fine scale solution for $\varepsilon = 1/80$ together with its cell-average. Notice that the jumps at the interface are higher in regions where $u$ is closer to zero. This is due to (28). The differences are getting smaller as the non-wetting phase saturation increases.

As we can also see in the right picture of Figure 7, the solution inside each layer is not constant. This is contradicting (29), used in the derivation of the effective model, and meaning that the first term in the asymptotic expansion of the saturation (22) is not layer-wise constant. This difference can be explained by the fact that the computed solution incorporates also $O(\varepsilon)$ effects. These effects will vanish as $\varepsilon \searrow 0$, yielding piecewise constant solutions.

The comparison of the effective and the averaged fine scale solution for different times is shown in Figure 8. It can be seen that in both cases, since we start our numerical experiments with a fully oil saturated domain, the saturation does not drop below the macroscopic residual saturation $U^*$. This value represents the maximal amount of oil that will be trapped due to micro scale heterogeneities. On the micro scale, this is caused by the fact that there is no oil flow from a coarse layer into a fine one, unless the oil saturation in the coarse layer exceeds the entry point $u^*$. At the macro scale, this translates into effective convection.
Figure 6: Effective saturation (solid) computed assuming $p_c^1$ – continuous, and averaged saturations at $t = 0.8$.

Figure 7: Micro scale problem: oscillatory (solid) and averaged (dashed) oil saturation at $t = 0.8$, full (left) and zoomed view (right).
and diffusion vanishing on the interval \([0, U^*]\).

One can also notice a slightly less good agreement in the region where the solution is close to \(U^*\). This can be explained by the higher amplitude in the oscillations, encountered - as mentioned above - for such values of the averaged solution. But taking into account also the front region, as well as its velocity, we conclude that the two solutions are matching well in both qualitative and quantitative sense. In consequence, we consider the effective model derived assuming the continuity of \(p_c^1\) to be more appropriate than the one in [5], in particular for the flow regimes that are not dominated by diffusion.

![Graph showing upscaled and averaged solution](image_url)

**Figure 8:** Upscaled and averaged solution, \(t = 0.2, 0.5,\) and \(0.8\).

### 5 Final Remarks

We have derived an upscaled equation for a periodically layered medium. In doing so we have employed the method of homogenization. Trapping effects that appear on the micro scale due to the difference in the entry pressure corresponding to a homogeneous layer are explicitly taken into account. The resulting effective model is a nonlinear parabolic problem of degenerate type, incorporating convection. The effective functions can be seen as weighted harmonic means of the corresponding micro scale ones. These functions vanish whenever the effective saturation \(U\) is below \(U^*\), representing the maximal amount of trapped oil.

It has to be stressed that these results are only valid for moderate capillary numbers (\(N_c = O(1)\)). For different regimes, i.e. \(N_c = O(\varepsilon^n)\), the homogenization approach will lead to equations of different type (see, e.g. van Duijn et al. [5]).
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