Direct simulations of two-phase flow on micro-CT images of porous media and upscaling of pore-scale forces

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Abstract
Pore-scale forces have a significant effect on the macroscopic behaviour of multiphase flow through porous media. This paper studies the effect of these forces using a new volume-of-fluid based finite volume method developed for simulating two-phase flow directly on micro-CT images of porous media. An analytical analysis of the relationship between the pore-scale forces and the Darcy-scale pressure drops is presented. We use this analysis to propose unambiguous definitions of Darcy-scale viscous pressure drops as the rate of energy dissipation per unit flow rate of each phase, and then use them to obtain the relative permeability curves. We show that this definition is consistent with conventional laboratory/field measurements by comparing our predictions with experimental relative permeability. We present single and two-phase flow simulations for primary oil injection followed by water injection on a sandpack and a Berea sandstone. The two-phase flow simulations are presented at different capillary numbers which cover the transition from capillary fingering at low capillary numbers to a more viscous fingering displacement pattern at higher capillary numbers, and the effect of capillary number on the relative permeability curves is investigated. Overall, this paper presents a new finite volume-based methodology for the detailed analysis of two-phase flow directly on micro-CT images of porous media and upscaling of the results to the Darcy scale.

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1. Introduction

Understanding immiscible two-phase flow through porous media is central to a number of industrial applications such as hydrocarbon recovery [7], CO₂ storage in underground reservoirs [30,42], and proton exchange membrane fuel cells [23,43,56]. These types of flow are usually driven by forces such as rock adhesion (wettability), gravity or due to pressure gradients caused by pressure differences on the boundaries of the flow domain. Viscous forces, on the other hand, are always resistive forces, trying to slow down the flow. The balance of these forces control the pore-scale processes, and determine the macroscopic behaviour of the flow.

Core-scale laboratory experiments [1,3,25,35] are commonly used to obtain the macroscopic properties of flow through porous media. This is usually achieved by measuring the flow parameters, such as pressures and flow rates on the boundaries of core samples, often complemented with imaging the location of the fluid phases inside the pore space [1,32]. These experiments can be used to obtain relative permeability and capillary pressure curves and residual saturations. However, laboratory measurements are costly and time consuming and, more importantly, extracting the necessary information to describe macroscopic flow accurately is not trivial. For example, it is difficult to measure the capillary and viscous pressure drops from a single experiment; see for example Hou et al. [25].

Pore-network models have been extensively used to study multiphase flow through porous media [2,6,10,11,15,16,27,37,39,51,55]. In pore-network models, the main structure of the pore space is represented by a network of pores connected by narrower restrictions (throats), and the flow through the network is modelled using analytical relations to describe the flow for each element of the network. Pore-network models have been used to predict relative permeabilities obtained from laboratory measurements [2,12,37,39,51,55]. However, there are still open questions on the predictive capabilities of the current pore-network models due to over-parametrization of available network extraction and modelling work-flows [52]. In particular these codes have two main limitations: (1) they do not naturally accommodate all the forces at the pore scale, being entirely quasi-static or including viscous effects as a perturbation, see Joekar-Niasar and Hassanizadeh [29] for a review; and (2) they simplify the pore structure and so do not accurately capture pore-body filling processes.

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With the advent of network models, specifically dynamic network models which do not assume capillary equilibrium during the displacement process, there has been a significant effort to find the link between the pore-scale pressure and the Darcy-scale pressure drops; see Korteland et al. \[31\] and Gray et al. \[20\] for recent reviews on the subject. For homogeneous porous media at the core scale, assuming a representative elementary volume (REV) exists, traditionally the intrinsic phase-volume weighted average pressure has been used \[31\]. Extensions to this averaging scheme have been developed for the cases where subscale heterogeneities in material properties or fluid distribution exist, for example by Nordbotten et al. \[34\] who propose a higher order approximation to the subscale pressure as opposed to the zero order approximation achieved by the traditional phase-volume averaging scheme.

More recently, detailed simulation techniques which simulate the flow directly on the micro-CT images of porous media have been conducted using lattice-gas/Boltzmann methods \[13,18,38,40,47,49\] and the level set method \[28,41\]. In addition, volume-of-fluid based finite volume methods have been used to model two-phase flow on two-dimensional images of porous media \[17,26\]. The advantage of direct methods is that they can accommodate viscous and capillary forces while preserving the pore-space geometry. However, these methods are computationally more expensive, and limited to small image sizes – typically a few millimetres across – and relatively high capillary numbers – usually higher than \(10^{-5}\). Calculating the Darcy-scale pressures from these simulations, however, is challenging due to large pressure variations and discontinuities in fluid phases at small scales.

In this paper, we present direct single and two-phase flow simulations on sample micro-CT images of porous media, a Berea sandstone and a sandpack called LV60A \[15\]. The flow equations are solved using a volume-of-fluid based finite volume method, with a new filtered surface force formulation \[45\] developed for efficient modelling of two-phase flow at low capillary numbers. Each of the pore-scale (defined here as the scale of grid-blocks used to discretize the pore-space) forces – viscous, dynamic pressure gradient, interfacial force and capillary pressure gradient – is obtained separately from the numerical solution of the Navier–Stokes equation and from the Poisson equation for capillary pressure. We present a rigorous methodology to upscale the pore-scale forces to obtain the Darcy-scale viscous pressure drops, based on an analogy of the Darcy equation with the energy conservation law (Section 2). In this approach, the Darcy-scale viscous pressure drops in individual phases are defined as the rate of energy dissipation per unit flow rate of each phase \[21,54\]. We verify this approach by using it to obtain the pressure drop in single-phase flow simulations from the pore-scale forces and compare the results with the conventional approach for obtaining the pressure drop – subtracting the upscaled pressures of the inlet and outlet boundaries (Section 4). Then, we present two-phase flow simulations for primary oil injection (Section 5) followed by water injection at two capillary numbers (Section 6) and use the proposed upscaling approach to obtain the pressure drops and the relative permeability curves from these transient two-phase flow simulations. The importance of this upscaling approach is that it allows the pressure drops to be calculated for relatively small volumes of porous media and for the cases where a phase is not connected to inlet or outlet boundaries, where it is otherwise difficult to calculate the upscaled pressure drops accurately due to the non-uniform fluid distributions along the flow domain and large spatial variations of the fluid phase pressures on the inlet and outlet boundaries. Finally, in Section 7, we compare our predictions with experimental relative permeabilities to verify our numerical method and show that the proposed upscaling approach is consistent with the conventional approach used for defining/measuring the pressure drops in laboratory two-phase flow experiments.

2. The relation between micro-scale forces and Darcy-scale pressure drops

In the following, we first describe the Navier–Stokes equations used to describe flow at the pore scale, which are solved using a new formulation optimised for modelling two-phase flow at low capillary numbers. Then, we briefly discuss the Darcy equation which is used in the macroscopic description of the flow. In Section 2.3, we show how the pore-scale forces used in the Navier–Stokes equations can be upcaled to obtain the Darcy-scale pressure drops.
2.1. Pore-scale description of flow

At the pore scale, the momentum balance equation for incompressible fluids is used to relate the pressure gradient, inertial, capillary, gravity and viscous forces. Knowing the pressure gradient, capillary and gravity forces, the momentum balance equation can be used to update the velocity field at any time-step:

$$\frac{D}{Dt}(\rho \mathbf{u}) - \nabla \cdot F = -\nabla p_{\text{d}} + \rho \mathbf{g} + \mathbf{f}_c - \nabla p_{\text{c}},$$

(1)

where $\mathbf{u}$ is the velocity vector, $\frac{D}{Dt}(\rho \mathbf{u}) = \frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u})$ is the inertial term, which accounts for acceleration of the fluid and momentum transfer due to advection. $T = \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ is the viscous stress tensor. For the case of incompressible two-phase flow, $\nabla \cdot \mathbf{u}$ can be written as [see (50) for the derivation]:

$$\nabla \cdot \mathbf{u} = (\mathbf{u} \cdot \nabla) \mathbf{u}.$$

(2)

The dynamic pressure field, $p_d$, can be obtained by solving the mass balance equation for incompressible flow:

$$\nabla \cdot \mathbf{u} = 0,$$

(4)

which is combined with the momentum balance equation (Eq. (1)) to obtain an equation for $p_d$, see [45] for more details. $\rho$ and $\mu$ are fluid density and viscosity, respectively, which are calculated using an indicator function ($\alpha$):

$$\rho = \alpha \rho_1 + (1 - \alpha)\rho_2,$$

$$\mu = \alpha \mu_1 + (1 - \alpha)\mu_2$$

(5)

In the volume-of-fluid method, the indicator function, $\alpha$, is defined everywhere in the flow domain and represents the volume fraction of one of the fluids in each grid cell. If the cell is completely filled with the first fluid then $\alpha = 1$ and if it is filled with the second fluid $\alpha = 0$. The indicator function is used to control the location of the interface. It is evolved with an advection equation of the form:

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{u}) = 0.$$

(6)

The capillary force ($\mathbf{f}_c$) can be computed as a body force [14],

$$\mathbf{f}_c = \sigma \kappa \mathbf{n}_x \delta_x,$$

(7)

where $\kappa = \nabla \cdot (\mathbf{n}_x)$ is the interface curvature and $\mathbf{n}_x$ is the normal to the interface:

$$\mathbf{n}_x = \frac{\mathbf{V}_X}{|\mathbf{V}_X|}.$$

(8)

The value of the $\alpha$ and $\mathbf{n}_x$ at the solid boundaries, however, are obtained using the contact angle, as discussed in [45]. Finally, $\delta_x$ is a delta function which has the shape of a Dirac delta function in the normal direction to the interface. By solving these equations (Eqs. (6), (3), (1) and (4)) we obtain the primary unknowns $\alpha$, $p_d$, $\mathbf{u}$ and $p_c$, respectively. We use the OpenFOAM [36] finite volume library to solve these differential equations. The details of the numerical implementation can be found in [44,45].

2.2. Macroscopic description of the flow

Large-scale flow through porous media is described by defining the macroscopic pressure and flow rates over a representative elementary volume (REV), where the REV-scale is the scale above which the heterogeneities at smaller scales do not affect these macroscopic properties [7]. The Darcy equation is then used to relate the flow rate to the macroscopic pressure drop ($\Delta P$), which for single-phase flow through a one-dimensional porous medium with a length of $\Delta x$ is as follows (in this paper we ignore the gravity force for the sake of simplicity):

$$V_0 = \frac{Q}{A} = \frac{K \Delta P}{\mu \Delta x},$$

(9)

where $V_0$ is the Darcy velocity, $Q$ is the flow rate (volumetric flux), $A$ is the cross-sectional area of the porous medium and $K$ is its permeability.

The REV concept is applied for field-scale simulation of multi-phase flow and the Darcy law is generalized to relate the flow rate of each phase ($a$) to the gradient of a macroscopic pressure for that phase ($\Delta P_a/\Delta x$):

$$V_{0,a} = -\frac{k_{r,a}K \Delta P_a}{\mu_a \Delta x}.$$

(10)

If we have two fluid phases – wetting ($a = w$) and non-wetting ($a = nw$), their macroscopic pressures are assumed to be related to each other using an equation of the form:

$$P_{nw} - P_w = P_c,$$

(11)

where $P_c$ is called the macroscopic capillary pressure, usually obtained from laboratory experiments.

Finally, $k_{r,a}$ is the relative permeability for fluid phase $a$, which is assumed to be a function of the phase saturations ($S_a$). It accounts for the additional pressure drop for each phase in a two-phase flow experiment, compared to a single-phase flow experiment at the same flow rate:

$$k_{r,a} = \frac{Q_{a,w}/\Delta P_a}{Q_{a,nw}/\Delta P_{nw}},$$

(12)

where $\Delta P_a$ is the macroscopic pressure drop in each phase, $a = w, nw$. $Q_a = \int \mathbf{u} \cdot \mathbf{n}_x dA$ is the flow rate passing through a cross section with area $A$ and $S_w = \alpha$ and $S_{nw} = 1 - \alpha$. The subscript $SP$ is used to indicate that the variable corresponds to the single-phase flow experiment.

2.3. Relation between pore-scale forces and corefield-scale pressure drops

The microscopic pressures, $p_d$ and $p_c$, are defined at each point in the flow domain, while the Darcy-scale pressures, $P_c$, are used to calculate fluid flow rates at larger scales. In any upscaling approach, there is a natural ambiguity in the definition of an upscaled (Darcy-scale) pressure, or upscaled pressure gradient, $\Delta P_a/\Delta x$, since it is not evident how the microscopic pressure should be averaged. In this section we propose an unambiguous definition of the Darcy-scale pressure gradient based on an energy conservation approach.

Let us first consider a control volume of an incompressible single-phase fluid in the pore space of a one-dimensional porous medium with a length of $\Delta x$, moving with the flow, with pore cross-sectional areas of $A_L(\equiv A_{phL})$ and $A_R$, and average pore velocities of $U_L(\equiv V_0/\phi_L)$ and $U_R$, at the left (inlet) and right (outlet) sides of the control volume respectively. Let assume that the pressure at the left side of the control volume is uniform and equal to $P_L$, and the pressure at the right side of the control volume is $P_R$, $\Delta P = P_R - P_L$, and the flow rate is $Q$. For such a system, during a period $dt$, the fluid at its left side moves a distance $dX_L = U_L dt$ and the fluid at its right side moves a distance $dX_R = U_R dt$. Forces equal to $P_L dA_L$ and $-P_R dA_R$ act at the left and right sides of the
control volume, respectively. Therefore, the work done on the fluid can be calculated as follows:

$$dW_p = P_l A_l U_l dt - P_l A_q U_q dt = (P_l - P_q) Q dt$$

(13)

For more general cases where $p$ and $u$ are not uniform at the inlet or outlet we have:

$$dW_p = \int_{A_l} P_l d\mathbf{x} dA_l - \int_{A_q} P_q d\mathbf{x} dA_q$$

$$- dW_p = \int_{A_q} P_q d\mathbf{x} dA_q - \int_{A_l} P_l d\mathbf{x} dA_l = (P_l - P_q) Q dt$$

Therefore, Eq. (13) is valid for these general cases as well, provided that we define the macroscopic pressures $P_l = \int P dA / Q$ and $P_q = \int P dA / Q$, where $u$ is the component of the velocity normal to $dA (u = \mathbf{u} \cdot \mathbf{n}_k$). In other words, when averaging the pressure over a cross-sectional surface, we have to weigh the pore-scale pressure by the flow rate passing through the surface. Therefore, for single-phase flow, we can write:

$$\Delta P = \frac{1}{Q} \frac{dW_p}{dt}$$

(14)

The energy is conserved. Consequently, in single-phase flow, the work done on the fluid by the pressure drop is dissipated by the viscous force, assuming that the inertial terms are negligible:

$$\left( \frac{dW_p}{dt} \right)_{\text{sp}} \approx - \left( \frac{dW_p}{dt} \right)_{\text{sp}}$$

(15)

where $\frac{dW_p}{dt}$ is the rate of dissipation of energy in the fluid due to internal viscous forces, which can be calculated as follows:

$$\Delta P_{\text{sp}} = \frac{1}{Q} \frac{dW_p}{dt} = \frac{1}{Q} \int_{V} (\mathbf{V} \cdot \mathbf{T}) \cdot d\mathbf{V}$$

(16)

The definition given above for the single-phase pressure drop has been used previously by Talon et al. [54] for the calculation of single-phase permeability from lattice-Boltzmann simulations.

In multiphase flow, the energy balance is more complex. The macroscopic pressure drops ($\Delta P_a, a = w, mw$), which are upscaled measures of pore-scale pressure gradients and driving forces ($-Vp_a + \rho g + f_e - Vp),$ are dissipated by viscous forces ($\mathbf{V} \cdot \mathbf{T}$). The macroscopic capillary pressure, on the other hand, results in additional exchange of energy with the interfacial energy as the fluid–fluid and fluid–solid interfaces grow and shrink. We use Eq. (16) to define the viscous pressure drops in two-phase flow as well. We define the viscous pressure drop in each phase as the rate of viscous energy dissipation per unit flow rate of that phase:

$$\Delta P_a = - \frac{1}{Q_a} \int_{V} (-Vp_a + \rho g + f_e - Vp) \cdot d\mathbf{V}_a$$

$$\approx \frac{1}{Q_a} \int_{V} (\mathbf{V} \cdot \mathbf{T}) \cdot d\mathbf{V}_a = \frac{1}{Q_a} \frac{dW_{\mu,a}}{dt}$$

(17)

where $V_a$ accounts for the portion of the flow volume occupied by phase $a$.

The above definition of pressure drop in individual phases is consistent with the definition of pressure drop in a continuous phase in steady-state relative permeability curves. The proof presented for Eq. (16) for the single-phase pressure drop is also valid for calculation of pressure drops in a continuous phase in a steady-state two-phase flow experiment, if we ignore the energy exchange between the two phases due to the viscous drag force at the interface [46].

The contribution of pore-scale forces to the Darcy-scale viscous pressure drops can be clarified by writing the mechanical energy-balance equation for the control volume. It can be derived by writing the dot product of the velocity vector and the momentum-balance equation (Eq. 1), and integrating it over the control volume:

$$\int_{V} \mathbf{u} \cdot (\mathbf{V} \cdot \mathbf{T}) dV = \int_{V} \mathbf{u} \cdot \left( \frac{D}{Dt} (\rho \mathbf{u}) + \nabla p_d - f_e + \mathbf{V} p_e \right) dV$$

(18)

Comparing this equation with Eq. (17), and ignoring the kinetic energy term, $\mathbf{u} \cdot (\frac{D}{Dt} (\rho \mathbf{u}))$, for slow flow, we can see that the viscous pressure drop is equal to the sum of energy introduced into the system by the capillary field ($f_e - Vp_e$) and the dynamic pressure gradient ($Vp_d$) forces per unit flow rate. This implies that both the dynamic pressure gradient and the capillary field contribute to the macroscopic pressure drop used in the multiphase Darcy equation. At the pore-scale however, the dynamic pressure gradient mainly stores information concerning the boundary conditions, while the capillary field depends on the equilibrium state of the interfaces and controls the phase distributions in the pore space.

Note that the above definitions do not require a definition for the macroscopic capillary pressure. The macroscopic capillary pressure drop can be defined in such a way to account for the difference between the energy introduced into the system at the boundaries and the energy dissipated by the viscous forces, which is equal to the changes in interfacial energy since the energy is conserved. Calculating the macroscopic capillary pressure from direct simulations is beyond the scope of this paper and will not be discussed further.

The viscous pressure drop obtained from Eq. (17) using the integral containing the viscous stress tensor, $\mathbf{T}$, is used in the following sections to calculate the pressure drops in individual phases which are in turn used in the calculation of relative permeability curves.

3. Micro-CT images and simulation parameters

The details of the images used in our simulation, the Berea sandstone and the LV60A sandpack, are given in Table 1. We use an unstructured mesh to discretize the flow domain, in which the grid blocks have the size of roughly 2³ voxels in big pores and 1 voxel in throats and corners.

In both oil-injection and water-injection simulations, a zero-gradient boundary condition is used for all variables, including pressure and velocity, at the outlet. We use a fixed average value boundary condition for the dynamic pressure ($p_d$) at the inlet, with the average value set to zero. The velocity boundary condition at the inlet is set to a relaxed-fixed injection rate of one phase – this boundary condition is designed to gradually move the injection rate toward the desired injection rate while keeping the velocity values as close as possible to a zero-gradient boundary condition. To start the simulations we initially fill a small portion of the image toward the inlet with the injected phase and the injection is done through the cells on the inlet boundary which remain filled with the injected phase. To ensure that there are always cells at the inlet containing the injected phase, we assign the inlet values of the indicator function by assuming that the angle between the fluid–fluid interface and the inlet is zero toward the injected phase.

In all simulations, the densities and viscosities of both fluids are equal and the same as of water at room temperature:

<table>
<thead>
<tr>
<th>Table 1</th>
<th>Details of the micro-CT images used in our simulations.</th>
</tr>
</thead>
<tbody>
<tr>
<td>LV60A</td>
<td>Berea</td>
</tr>
<tr>
<td>Size (voxels)</td>
<td>$282 \times 174 \times 174$</td>
</tr>
<tr>
<td>Voxel length</td>
<td>$8.2 \mu m$</td>
</tr>
<tr>
<td>Number of grid-blocks</td>
<td>$764,578$</td>
</tr>
<tr>
<td>Effective porosity</td>
<td>$36.1%$</td>
</tr>
<tr>
<td>Predicted permeability</td>
<td>$31.6$ Darcy</td>
</tr>
<tr>
<td>Experimental permeability</td>
<td>$32.0$ Darcy [53]</td>
</tr>
</tbody>
</table>
\[ \mu = 0.001 \text{ Pa s and } \rho = 1000 \text{ kg/m}^3. \] The contact angle used is zero during oil injection and 45° in all water-injection simulations, consistent with direct in situ measurements in a water-wet rock [5].

### 4. Validating the upscaling method for single-phase flow simulations

To validate the upscaling approach presented in Section 2.3, we use it to analyse steady-state incompressible single-phase flow simulations on the Berea and LV60A images discussed in the previous section. We use the same initial and boundary condition as the subsequent water-injection simulations, except that the flow domain is initially filled only with water. We analyse control volumes of the flow domain spanning from 20% to 90% of the simulations, to be consistent with the two-phase flow simulation results presented in the next sections. We compare different approaches for upscaling single-phase pore-scale forces to obtain the Darcy-scale pressure drop (\(\Delta p\)), as follows:

- **Option a**: subtracting area weighted average of inlet and outlet pressures:
  \[ \frac{1}{h_i} \int_{A_i} p dA_i - \frac{1}{h_o} \int_{A_o} p dA_o. \]

- **Option b**: subtracting flux weighted average of inlet and outlet pressures:
  \[ \frac{1}{h_i} \int_{A_i} u d\mathbf{A}_i - \frac{1}{h_o} \int_{A_o} u d\mathbf{A}_o. \]

- **Option c**: velocity weighted average of the pore-scale pressure gradient:
  \[ - \frac{1}{h} \int_{A} \nabla \cdot (p \mathbf{v}) dV. \]

- **Option d**: velocity weighted average of the viscous force:
  \[ - \frac{1}{h} \int_{A} \mathbf{u} \cdot (\nabla \cdot (p \mathbf{u})) dV. \]

- **Option e**: velocity weighted average of the pore-scale pressure gradient:
  \[ - \frac{1}{h} \int_{A} \nabla \cdot (\mathbf{v} p) dV. \]

Among the options above, Option a is the common approach for calculating and measuring pressure drop. If the size of the flow domain is significantly larger than the assumed REV, then the averaging can be done on REVs close to the inlet and outlet, in which case the approach is called the volume-weighted averaging of pressure [31,34]. This option also reproduces what is measured in a macroscopic experiment. Option b obtains the upscaled pressures on the image boundaries too; but it has the advantage that the upscaled pressures satisfy the energy-balance equation, as discussed in Section 2.3. Option c is identical to Option b for incompressible single-phase flow, which can be proved from the incompressibility condition, \(\nabla \cdot \mathbf{u} = 0\), and applying the Divergence theorem on \(\mathbf{u} \cdot \mathbf{v}\).

\[
\int_V \mathbf{u} \cdot (\mathbf{v} p) dV = \int_V \nabla \cdot (\mathbf{v} p \mathbf{u}) dV = \int_A p \mathbf{u} \cdot \mathbf{n} dA = \int_{A_i} p u dA_i - \int_{A_o} p u dA_o.
\]

The difference is that Option c up scales the pressure gradient force to obtain the pressure drop without first upscaling the pressure on the boundaries; this is a big advantage for analysing the two-phase flow simulations where the individual-phases may not be connected to both the inlet and outlet boundaries and where the fluid distribution and pressure profile is not uniform. Option d, which has been previously used by Talon et al. [54] to compute single-phase permeability from lattice-Boltzmann simulations, can be considered as an approximation to the pressure drops obtained by Options b and c for slow flow where inertial terms are negligible.

Finally, Option e is presented here to show that we will not obtain the Darcy-scale pressure gradient (\(\Delta p/\mathbf{A_t}\)) by applying the volume-weighted averaging to the pore-scale pressure gradient (\(\mathbf{v} p\)); by doing so we obtain an average force per unit volume which can be very different from the Darcy-scale pressure gradient. Nevertheless, as explained earlier, we can apply the volume-weighted averaging to the pore-scale pressure (\(p\)) over an REV to obtain the Darcy-scale pressure [31,34].

Table 2 summarises the results of the upscaling options above for the steady-state incompressible single-phase flow simulations on the Berea and LV60A images.

It is clear that the results from our velocity-weighted averaging approach presented in Section 2.3 (Options c and d) agree with those obtained by the conventional approaches, obtained by subtracting the upscaled outlet and inlet pressures (Options a and b). However, the results obtained from the volume-weighted averaging of the micro-scale pressure gradient force (Option e) show a significant deviation: the pressure drop is significantly underestimated, since large stagnant regions of the pore space have low pressure gradients; in a heterogeneous natural porous media the flow is accommodated in a few fast-flowing pathways [8,9]. This shows that the volume weighted average of pore-scale pressure gradient (which can be considered as the average force per unit area in the flow direction) cannot be considered as a measure of pressure drop. The results from the upscaling of the viscous force (Option d) are close to those obtained by directly upscaling the pore-scale pressure gradient force (Option c). The differences, which are roughly 3% of the viscous pressure drops, account for the energy dissipated due to the changes in fluid velocity, \(\frac{1}{h} \int_{A} \mathbf{u} \cdot (\nabla \cdot (p \mathbf{u})) dV\), and are equal to 70.0 and 8.9 Pa for the single-phase flow simulations on the Berea and LV60A images, respectively. The work done by the pressure gradient force (Option c) is equal to the sum of the viscous dissipation of energy (Option e) and the energy dissipated due to the changes in fluid velocity, per unit flow rate, which confirms that our method conserves energy as well.

In the rest of this paper we use Option d to calculate relative permeability, although similar results were obtained from Option c. The advantage of Option d, which is an approximation to the actual pressure drop (Options b and c), is that it does not have the contribution of the changes in kinetic energy and consequently it has a lower level of noise due to the sudden changes in the fluid velocity encountered in snap-off events in two-phase flow simulations. Options a and b, however, cannot be used accurately to obtain the pressure drops in our transient two-phase flow simulations due to discontinuity of fluid phases and large variations in the fluid phase pressures on the boundaries.

### 5. Primary oil injection

In the primary oil (non-wetting phase) injection simulations, we assume a contact angle of 0° between the grain walls and the fluid–fluid interface. Initially, we filled all the grid-blocks located in the first 8% of Berea and the first 13% of LV60A images with oil. Fig. 1 shows the flow domain for the two images at the beginning of the oil-injection simulations.

The oil-injection simulations on each image are performed at two capillary numbers of \(N_c = \frac{\mu}{\sigma} = 1.5 \times 10^{-5}\) and \(6 \times 10^{-5}\). Fig. 2 shows a comparison of the phase distributions in the pore space for the two capillary numbers after injecting 0.15 pore volumes of the non-wetting phase.
These visualizations indicate a transition from a capillary-fingering displacement pattern at low capillary numbers toward a viscous-fingering pattern (fingers developing along the main flow direction) at high capillary numbers \citep{33}. To obtain the relative permeability curves, we continued the simulation on LV60A for the capillary number of \( N_c = 6 \times 10^{-5} \) until two pore volumes of the non-wetting phase were injected. The simulations on Berea image for \( N_c = 1.5 \times 10^{-5} \) continued until one pore volume of the non-wetting phase was injected. Our preliminary analysis of the residual non-wetting phase saturations after imbibition simulations show that the effect of capillary number becomes important at relatively lower capillary numbers for the Berea sandstone compared to sandpacks \citep{44}, which is the reason we have chosen a lower capillary number for the simulations on the Berea compared to the LV60A sandpack.

The upscaling methodology presented in Section 2.3 is used to analyse control volumes in the flow direction, \( x \), from \( x = x_L \) to \( x = x_R \), cutting out all grid-blocks outside the interval \([x_L, x_R]\). \( x_L \) and \( x_R \) are chosen to exclude the first 20% and the last 10% of the images from the post-processing stage, to avoid boundary effects. Fig. 3 shows the results for the viscous pressure drops and relative permeabilities for the two images. As stated before, the pressure drops and the relative permeabilities are calculated using Eq. (17) and Eq. (12) respectively. Each point in these figures represents the average value over a time interval which is chosen in such a way to have similar number of points for each relative permeability curve. This averaging also helps to reduce the high frequency fluctuations introduced by the pore-scale events (Haines jump and snap-off) due to the small size of the image. Note that the pressure drop for the wetting phase at the end of simulations is not accurate as its flow rate is close to zero and Eq. (17) becomes sensitive to numerical errors.

The relative permeability results presented in Fig. 3 show that the wetting phase relative permeability at the end of the simulations is very low and close to zero. On the other hand, visualizations of the wetting phase at the end of the simulation, presented in Fig. 4, show that there are large clusters of the wetting phase connected to the outlet. This implies that if we continue the simulations for a longer period, the wetting phase saturation will decrease further. However, since flow through the wetting layers is slow, it takes a long time to reach a low wetting phase saturation. Moreover, our numerical method does not accurately capture layer flow through corners when the layer thickness is smaller than the grid-block size, and that may have biased the relative permeability results at the end of our simulations. Flow through such layers can be studied, for example, by using higher resolution
micro-CT images, or by incorporation of an additional film flow model to the direct numerical simulations. Modelling film flow at such small scales, however, is a complicated task as it requires information on the sharpness of the corners and the roughness of the solid walls and is a subject for future work.

6. Water injection

Drainage, presented in the previous section, is followed by water-injection simulations and the effect of capillary number on the displacement pattern during water injection is investigated. The contact angle used in all of our water-injection simulations is $45^\circ$ toward the water phase [5]. The other boundary conditions are the same as in the oil-injection simulations except that we swap the injected phase. The initial condition for the fluid phase distribution (indicator function) in water-injection simulations are taken from their distribution at the end of primary oil-injection simulations. The first 13% of the image toward inlet, however, is filled with the wetting phase and the wetting phase is injected through the inlet faces which are in contact with the wetting phase. Fig. 5 shows comparisons of the non-wetting phase distributions, during and at the end of the simulations, for two capillary numbers, for water-injection simulations on the LV60A sandpack and Berea sandstone.

The results presented in Fig. 5 show that, at lower capillary numbers, the wetting phase has sufficient time to flow through narrower flow paths (corners and narrower throats) leaving larger ganglia of the non-wetting phase behind, while as we increase the capillary number the flow becomes closer to piston-like displacement behaviour. Moreover, the trapped ganglia become smaller as we increase the capillary number. This observation could be explained by the criterion presented for the mobilization of oil droplets in [46,48]. The criterion states that the maximum capillary field in a non-wetting phase droplet is inversely proportional to the droplet size. Therefore, at higher capillary numbers, the size of the droplet should be smaller, so that the capillary field inside the droplet ($\nabla P_{nw}$) would be greater than the sum of the dynamic pressure gradient force ($-\nabla P_{nw}$) and the viscous drag force between the two phases.

Similar to the oil-injection simulations, we have analysed control volumes of the flow domain spanning the interval from 20% to 90% of the images. Fig. 6 shows the results for viscous pressure drops (Eq. (17)) and the corresponding relative permeability curves (Eq. (12)).
There are small errors in the numerical results, but as it can be seen at the end of our imbibition simulations the non-wetting phase relative permeability converges to zero, which implies that the remaining non-wetting phase at the end of the simulations is trapped. However, at the beginning of the imbibition simulations the water relative permeability does not start from zero. This has a physical meaning that we have not continued our drainage simulations long enough to reach the immobile water saturation. The water relative permeability starts from a higher value for the simulations at higher capillary numbers (Berea simulations at $N_c = 6 \times 10^{-5}$ and LV60A simulations at $N_c = 1.5 \times 10^{-4}$), which is because the capillary number is changed from its previous value used in the drainage simulations.

Our visualizations of the non-wetting phase (Fig. 5) show that the pressure drops in individual phases are not uniform and therefore it is not always possible to define the pressure drops as the difference of the inlet and outlet pressures. In contrast the upscaling approach presented in this paper allows us to calculate them without ambiguity to obtain the relative permeability curves for relatively small image sizes.

7. Comparison with experiments

There is a significant amount of relative permeability data in the literature for Berea sandstone. Amaefule and Handy [4] presented steady- and unsteady-state relative permeability curves for oil–water systems and studied the effect of surface tension. Fulcher et al. [19] studied the effect of flow rate, viscosity and interfacial tension on steady-state relative permeability curves for different oil–water systems. Oak [35] presented steady-state two- and
three-phase relative permeability curves for gas–oil–water systems. In the absence of relative permeability curves for the specific rock sample on which we have performed our simulations, we present a comparison of our simulation results with these experimental relative permeability measurements on Berea sandstone in Fig. 7. More recently, Krevor et al. [32] have reported CO$_2$-water drainage relative permeability curves and Akbarabadi and Piri [1] have reported CO$_2$-water drainage and imbibition relative permeability curves. We present a comparison of our simulation results with these measurements too.

The drainage simulations used here are the same as those in Section 5. However, our imbibition simulation results are presented for a capillary number of $7.5 \times 10^{-5}$, which are run using the same boundary and initial conditions as those discussed in the previous section, except the initial condition for the indicator function where in this simulation we have only filled the first 4% of the image with the wetting phase. The modification of the initial condition for this simulation is introduced to avoid the interference of relatively high currents that arise due to the initial capillary non-equilibrium of the two fluids. The imbibition relative permeability curves for both phases are slightly lower than those presented in Fig. 6 for a higher capillary number of $1.5 \times 10^{-5}$. This shows that the effect of capillary number, although small, is still present in these results and further reducing the capillary number can affect the relative permeability curves. The imbibition relative permeability curve for the non-wetting phase is also plotted for control-volumes of the flow domain from 20% to 55% of the image, and from 55% to 90%, to show the sensitivity of our results due to boundary effects and control volume size. The relative permeabilities obtained for the second half of the image, which are further away from the inlet boundary, are in a better agreement with experimental measurements. This suggests that our results are

Fig. 6. Plots of upcaled viscous pressure drops in individual phases as a function of time (left column), and the corresponding relative permeability, for control volumes spanning from 20% to 90% of the images at the capillary numbers indicated.
and fluid properties, such as contact angle, as well as numerical properties, the dependence of relative permeability curves on rock millimetre to centimetre scale. These uncertainties in the rock dynamic micro-CT imaging of the multiphase displacement and calculations of flow can be used in conjunction with recent advances in measurements. Nevertheless, these results show that direct simulations to develop or validate new macroscopic models, which are computationally less expensive for modelling two-phase flow at low capillary numbers. In addition, application of direct numerical simulations to develop or validate new macroscopic models, which have been recently introduced to describe multiphase flow under a wide range of flow conditions through the introduction of non-equilibrium effects [22,24], can be considered in future work.

8. Conclusions

We have presented direct two-phase flow simulations on micro-CT images of a sandstone and a sandpack for primary oil flooding followed by water injection. We presented the water injection simulations at different capillary numbers which show the transition from capillary fingering at low capillary numbers to a more viscous fingering displacement pattern at higher capillary numbers. The pore scale forces were upscaled to obtain the Darcy-scale pressure drops using an energy balance concept. In this new approach, the pressure drops in individual phases are defined as the rate of viscous dissipation of energy in each phase per unit flow rate of that phase. We used this upscaling approach to obtain the relative permeability curves from our simulations and compared them with experimental measurements from literature, which show a good agreement considering the wide scatter in the experimental data due to different fluid/rock properties.

In summary, the results presented in this paper show that the direct simulation on micro-CT images can be used to understand the mechanisms controlling two-phase flow through porous media and to obtain Darcy-scale properties, such as relative permeabilities and residual saturations. Our numerical method provides a basis for further understanding of the role of various fluid/rock parameters such as contact angle and pore-geometry on the Darcy-scale properties of porous media. Moreover, higher-resolution direct numerical simulations can be used to create benchmark data for validating pore-network models, which are computationally less expensive for modelling two-phase flow at low capillary numbers. In addition, application of direct numerical simulations to develop or validate new macroscopic models, which have been recently introduced to describe multiphase flow under a wide range of flow conditions through the introduction of non-equilibrium effects [22,24], can be considered in future work.

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