Upscaling from pore to core: effects of strong capillary forces and wettability phenomena

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J. P. du Plessis Department of Applied Mathematics, Stellenbosch University, South Africa **ABSTRACT:** In the upscaling process from pore to core different techniques are being used. In this presentation a novel application of Volume Averaging is described. The basic development follows the representative unit cell concept (RUC) developed by du Plessis (1988). This RUC concept is extended to multiphase flow. With the aid of a conceptual geometrical micro-model of a porous medium effective equations are derived which describe multiphase flow. Due to the strong nonlinearity of the flow process non-local terms are introduced into the equations. These upscaled equations are analyzed in the presence of strong capillary forces and different wettability conditions inside the porous medium. The presence of capillary forces modifies the flow behaviour strongly and introduces non-local terms in the averaged equations.

LIST OF SYMBOLS

- \mathcal{A} : area in pore (corner) occupied by fluid $[m^2]$
- C : factor depending on x
- d : microscopic characteristic length (RUC) [m]
- f : Fanning friction factor for fully developed flow [-]
- $f(\theta, \delta)$: function describing geometric components, fig. 1b. [-]
 - g : gravity acceleration $[m/s^2]$
 - I : vector integral expression
 - k : number of corners in channel [-]
 - l_g : flow length inside RUC [m]
 - \mathcal{L} : length of interface [m]
 - n : fraction of porosity occupied by liquid or gas [-]
 - p : pressure $[kg/ms^2]$
 - q: volumetric flow rate $[m^3/s]$
 - Q: specific discharge over RUC (summed over individual corners) $[m^3/s]$
 - r : radius of curvature of gas-liquid interface [m]
 - r_{crit} : critical radius of curvature of gasliquid interface during drainage [m]
 - r_i : critical radius of curvature of gasliquid interface during imhibition [m]
 - r_h : hydraulic radius, [m]

- Re : Reynolds number, $\rho v_p D_h / \mu$, [-]
- S : surface $[m^2]$
- v : velocity [m/s]
- V_0 : volume of averaging volume $[m^3], d^3$
- β : resistance factor [-]
- δ : angle of corner *rad*
- ϵ : porosity $[m^3/m^3], V_p/V_0$
- γ : surface (interfacial) tension at inter-face $[kg/s^2]$
- ρ : density $[kg/m^3]$
- μ : dynamic viscosity [kg/ms]
- $\theta~$: contact angle liquid solid rad
- ν : normal vector on $\mathcal{S}[-]$
- subscripts:
- : gas
- l : liquid
- p : pore
- s : solid
- symbols:

 $\langle () \rangle$: average of quantity

- $\dot{()}$: deviation from mean
- || : streamwise pores
- \perp : transverse pores

INTRODUCTION

Multiphase flow through a porous medium has applications in many areas of science and engineering. Examples are unsaturated zone hydrology, petrophysics and catalytic flow reactors in chemical engineering. In this presentation the method of *Volume Averaging* is used to describe the behaviour of a wetting liquid inside a porous medium with the presence of a non-wetting liquid. Volume averaging has been used in the last decennia, mostly for single-phase flow in porous media, although examples of multiphase flow are described in (Bear & Bensabat 1989). Despite the enormous theoretical developments, up to now the practical applications of volume averaging have been limited due to the so called closure problem. Different possibilities exist to solve this closure problem: numerical methods (Quintard & Whitaker 1990), approximations based on empirical equations (Whitaker 1980) and analytical solutions for prototype unit cells (du Plessis & Masliyah 1988). The approach taken in this paper is based on the closure scheme developed in (du Plessis & Masliyah 1988). This scheme is augmented with additional boundary conditions which are introduced due to fluid-fluid interfaces. This has become possible due to the recent work of (Zhou, Blunt, & Orr, Jr. 1997), who derived an analytical approximation for the resistance factor to flow in corners.

THE BASIC INTERSTITIAL EQUATIONS

As a basis we start with the steady-state Navier-Stokes equations inside the pores of a porous medium. These equations are then averaged over a Representative Elementary Volume (REV). To make this possible the REV is modelled as a typical configuration of the pore space, called a Representative Unit Cell (RUC). For each of the fluid phases, e.g. gas and liquid, these equations are:

$$\nabla \cdot (\rho v v) = \rho g + \nabla p - \mu \nabla^2 v \tag{1}$$

They are augmented by the mass conservation equations:

$$\nabla \cdot v = 0 \tag{2}$$

with boundary conditions:

$v_g = 0$	at gas-solid interface	(3)
$v_l = 0$	at liquid-solid interface	(4)
$v_g = v_l$	at gas-liquid interface	(5)
$\left. \left(p_g - p_l \right) \right _x = \gamma$	$\gamma_{gl}C _x$ in longitudinal direction of capillary	(6)

The last boundary condition describes the surface forces acting on the fluids. It is assumed that the only surface force is surface tension, which is modeled by the Young-Laplace equation. If the fluid contents vary slowly in the longitudinal direction of the capillary (see region C of figure 2), the pressure of the non-wetting liquid is assumed constant and taken as reference pressure, the pressure in the wetting phase becomes:

$$p = -\frac{\gamma}{r} \tag{7}$$

Only the equations describing the liquid movement will be retained.

VOLUME AVERAGING FOR VARIABLE FLUID VOLUME FRACTIONS

In the literature several examples exist of the use of volume averaging inside a porous medium with constant volume fractions of fluids inside an averaging volume. Averaging with variable fluid fractions is not common and introduces extra terms in the averaged equations which are similar to the case when the porosity varies. The volume averaged form of equation (1) for the liquid is:

$$\rho_{l}\nabla\cdot(\epsilon n_{l}v_{ln}v_{ln}) = \epsilon n_{l}\rho_{l}g + \epsilon n_{l}\nabla p_{ln} + \mu_{l}\nabla^{2}(\epsilon n_{l} v_{ln}) - \rho_{l}\nabla\cdot(\epsilon n_{l}\langle\dot{v}_{l}\dot{v}_{l}\rangle_{n}) + \frac{1}{V_{0}}\int_{\mathcal{S}}\left(\nu\dot{p}_{l} + \mu_{l}\frac{\partial}{\partial\nu}(v_{l})\right) d\mathcal{S}$$

$$(8)$$

The surface integral terms have two contributions: from the gas-liquid and from the liquid-solid interface. Rearranging equation (8), dropping the terms containing momentum advection and convective terms and writing terms which generate momentum left and dissipate momentum right results in the following steady-state equation:

$$\epsilon n_l \rho_l g + \epsilon n_l \nabla p_{fn} = -\frac{1}{V_0} \int\limits_{\mathcal{S}} \left(\nu \dot{p}_l + \mu_l \frac{\partial}{\partial \nu} (v_l) \right) \, d\mathcal{S} \tag{9}$$

MODELLING OF THE VOLUME AVERAGED EQUATIONS

In order to find a simple approximation or analytical solution to the closure problem the integral terms in equation (9) have to be rewritten in explicit terms. The RUC concept of (du Plessis & Masliyah 1988) has to be changed to accommodate the specifics of gas-liquid flows. Flow channels are approximated by triangular channels. This is necessary in order to accurately model the saturation vs. capillary pressure relationship of porous materials. The wedge like corners of the triangular capillary allow for both fluid phases to be present in the pore simultaneously. The triangular pores are modelled as composed of right-angled triangles. These fit into corners of the RUC (figure 1).



Figure 1: a) Geometry of RUC. b) Geometry of interface between liquid and gas inside a corner, the direction of flow is perpendicular to the paper.

The geometrical properties \mathcal{L}_{gl} , \mathcal{L}_{sl} and $\mathcal{A} = f(\theta, \delta) r^2$ can be expressed in terms of r, δ and θ .

Capillary pressure relationship

The relation among pressure difference between the fluids and saturation is modelled similar to (Mason & Morrow 1991) using the MSP method. The major difference is that also the longitudinal changes in the fluid gas interface have to be approximated and that different contact angles are

taken into account. The derived relationship does not take into account the effects of surface adhesion forces, but could be modified accordingly.

If a non-wetting fluid enters a pore filled with a wetting fluid, an interface between the two fluids is formed. This interface is called a MTM (Main Terminal Meniscus). As soon as the two principal radii of the meniscus have the same magnitude, the non-wetting fluid enters the capillary. This radius is called the critical radius for drainage, r_{crit} . During imhibition, when a wetting fluid fills a capillary a different critical radius corresponds to complete filling of the capillary with the wetting fluid. This radius r_i corresponds to the case when the liquid from the separate corners starts to touch each other. r_{crit} is always smaller than r_i . Both of these critical radii depend on the contact angle. If there are saturation gradients along a pore, the average saturation inside the pores is calculated using the saturation profile given by (Dong & Chatzis 1995):

$$n_l = \frac{3f(\theta, \delta)l_g\gamma^2}{5V_p} \frac{p_l^{-5} - p_0^{-5}}{p_l^{-3} - p_0^{-3}}$$
(10)

Flow resistance relationships

In order to find an approximate analytical solution for the closure problem, the resistance to flow in the RUC channel needs to be specified. In case the channel is filled with one fluid only, standard solutions from (Shah & London 1978) are available. For two-phase flow the solution procedure from (Zhou, Blunt, & Orr, Jr. 1997) is followed.

These relationships are valid for laminar flow. The assumption of laminar flow is generally valid in the regime of slow two-phase flow. The flow resistances are written in terms of dimensionless resistance term β and the geometrical properties of the flow itself for the two-phase flow. The derivation of the resistance factors for two-phase flow is mainly based on the work of (Zhou, Blunt, & Orr, Jr. 1997) and (Mogensen & Stenby 1998). In contrast to single-phase flow, where fRe is given for the whole capillary, in two-phase flow the resistance factor is given for each corner in the capillary separately. The following describes the methodology for one corner at first. Inside the corner for the volumetric flow rate is defined as:

$$q_c = \frac{\mathcal{A}r^2}{\beta\mu_l}\nabla p \tag{11}$$

r depends on the capillary pressure and β is defined as in (Mogensen & Stenby 1998).

Modelling of the surface terms

In order to solve the closure problem, the integral term in equation (9) needs to be expressed in terms of the resistance factors and geometric terms. The surface integral in equation (9) can be split in the parts containing the liquid-solid interface and the liquid-gas interface. These two terms give the stress components. The tangential stresses at the gas-liquid interface are assumed to be zero, but because of the capillary effects, normal stresses do exist.

$$\mathbf{I}_{\mu} = \frac{1}{V_0} \int_{\mathcal{S}_{sl}} \left(\mu_l \frac{\partial}{\partial \nu} (v_l) + \nu \dot{p}_l \right) \, d\mathcal{S} + \frac{1}{V_0} \int_{\mathcal{S}_{gl}} \left(\mu_l \frac{\partial}{\partial \nu} (v_l) + \nu \dot{p}_l \right) \, d\mathcal{S} \tag{12}$$

To evaluate the above integral expression, the following assumptions are made:

- 1. The geometry is given by the RUC shown in figure 1.
- 2. The mean pore velocity v_p is directed axially along that specific pore section.
- 3. Pore sections (and thus also corners) are oriented perpendicularly and transversally with respect to the local average velocity.

- 4. The shear stress on the liquid is a function of fRe which in turn depends on the resistance factor β . The mass flow is constant in each capillary and the two terms which generate momentum for dissipation are the gravity term and the pressure term.
- 5. Normal stresses at the interface between the liquid and the gas are given by the Young-Laplace equation.
- 6. The form of the interface in longitudinal direction is modelled as in (Dong & Chatzis 1995). This implies that the volume averaged equation is valid inside region C (figure 2). Inside region A a the saturated case is recovered.



Figure 2: Regions where solution is valid (A, B); A: saturated, B: region of MTM $[r \ge r_{crit}]$, C: two-phase region $[r \le r_{crit}]$.

The integral term in equation (12) is rewritten using the conditions stated above:

$$\mathbf{I}_{\mu} = \frac{\mathcal{S}_{sl}\,\mu_l\,v_p\,f\mathrm{Re}}{8r_h V_0} \tag{13}$$

 $S_{sl}, v_p, f \text{Re}, r_h$ still depend on the boundary conditions p_0, p_l .

COMBINATION OF THE VOLUME AVERAGED EQUATIONS

If all volume averaged terms are used and the expression for \mathbf{I}_{μ} are substituted in equation (9), rearranged and rewritten in terms of p_0, p_l :

$$Q = -\left[\sum_{j=1}^{k} \frac{f_j(\theta, \delta)}{\beta_j}\right] \frac{16\gamma^4}{25\mu_l} \frac{(p_l^{-5} - p_0^{-5})}{(p_l^{-4} - p_0^{-4})} \left(\nabla p_{fn} + \rho_l g\right)$$
(14)

The summation term inside the square brackets is a purely geometric term, which is constant for a specific RUC chosen. Equation (14) contains no specific reference to the length scales of the RUC anymore. The length scale terms are implicitly contained in the boundary conditions p_0 and p_l . These boundary conditions together with the gradient term depend on the flow itself.

Equation (14) is an *"effective"* equation in terms of its parameters and the RUC scale. This equation has a non-local structure due to the incooperation of boundary conditions. The first part of equation (14):

$$\left[\sum_{j=1}^{k} \frac{f_j(\theta, \delta)}{\beta_j}\right] \frac{16\gamma^4}{25\mu_l} \tag{15}$$

contains only porous media and fluid dependent properties. The influence of wettability can be examined parametrically from equation (15)



Figure 3: a) Example solution of eq. (15), b) influence of contact angle on flow resistance. (scaled).

Example

In figure (3a) the combined influence of corner angle δ and contact angle θ on the flow resistance is shown. Figure (3b) shows that when $\theta \leq \frac{\pi}{6}$, the flow resistance strongly increases.

CONCLUSIONS

The volume averaged form of the transport equation for two-phase flow has a different structure than the single-phase equation. The most significant is the introduction of boundary conditions in the equation itself. The influence of wettability is strongest in pores with small corner angles. This together with the marked influence of capillary pressure leads to increasingly higher flow resistance. A point of further research is the specification of external boundary conditions. Because the volume averaged nature of the equations, also the boundary conditions need to be volume averaged.

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