SIMULATION OF SINGLE AND TWO PHASE NEWTONIAN FLOW IN CARBON CAPTURE AND STORAGE PROCESSES USING VARIATIONAL METHODS

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Abstract

Variational method is a promising way to study the kinetic behavior and storage potential of carbon dioxide (CO_2) at the porous scale in the presence of other phases. The current study validates variational solutions for single and two-phase Newtonian flow through angular pores for special geometries whose analytical and/or empirical solutions are known. The hydraulic conductance for single phase flow through a triangular duct was also validated against empirical results derived from lubricant theory. The variational method predicted flux and hydraulic conductance through the chosen geometries within 2-5% error with one parameter, and <2% for two parameter in circular geometry ratio of inner to outer radius <0.2). The results of this study indicate that this technique can potentially be applied to non-Newtonian and multiphase flow, and flow domains with irregular geometries. This provides a powerful technique for pore-scale network modeling of carbon sequestration reservoir flow.

I. Introduction

CO2 reservoir storage and enhanced oil recovery schemes are the net result of fluid transport at the microscopic level (Sholokhova, 2009). However, high resolution simulations of these schemes are often hindered by high computational costs (Babaei & King, 2010). The detailed mathematical description of geophysical phenomena at the porous level leads to complexities whose simulations cannot be resolved within reasonable time constraints for large scale reservoir simulations (Abate et. al. 1999). These complexities are generally resolved by implementing macroscopic continuum models of fluid flow through porous media, such as the Ergun Equation or Darcy's Law (Ertekin, 2001). These models operate under the assumption of negligible heterogeneities with respect to the scales of the porous media under consideration (Sochi, 2007). Consequently, the microscopic complexities of pore structure are often condensed in terms of single parameters such as porosity and permeability (Sochi, 2007). Furthermore, homogeneity of these parameters is generally assumed to be uniformly distributed over large spatial regions (Ghomian, 2008). The net effect of this averaging is computationally efficient simulation with low resolution physics.

The need to balance pore-level physics and macroscopic scaled reservoir simulations has lead to an alternative approach: Pore-Network Models (Sochi, 2007). The effectiveness of these models is contingent upon the development of computationally efficient methods for resolving physical parameters at the pore scale (Sholokhova, 2009). Hydraulic conductance, a crucial ingredient to the prediction of permeability and relative permeability, is one of the parameters which must be resolved at the pore level. Its dependence on the fluid velocities derived from solutions to Euler's equations implies that a variety of numerical methods for solving partial differential equations can be employed. The variational method presents a powerful method for high resolution hydraulic conductance in various pore channel shapes.

The current study validates the use of the variational method to compute hydraulic conductance of single and two phase Newtonian flow through simple geometries, relevant to pore network modeling. The chosen pore geometries provide analytical and/or empirical hydraulic conductance solutions for verification purposes.

II. Variational Method

In a straight channel or for a weakly converging-diverging geometry by way of the lubrication approximation, the flow velocity $w_i(x,y)$ at a point (x, y) in the cross section satisfies the following Poisson equation

$$0 = G + \mu \nabla^2 w$$

for one phase flow where G is the pressure gradient per unit length, μ is the kinematic viscosity, and w is the axial velocity. Define a function (I[f]): $I[f\ ] = \frac{1}{2}\int_R dxdy\{\mu\ \nabla f\ \nabla f\ - 2G\ f\ \}$

Its minimization, which also corresponds to minimizing total energy, satisfies

$$I[f\ ] \geq -\frac{1}{2}Gq$$

is used to find the parameter α. Here, f is a test function that satisfies the boundary conditions and weakly approximates the solution to Poisson equation.

The flux (q) and hydraulic conductance (g) is given by $q\ = \int_R dxdyw\ \ and\ g = \frac{q}{G/\mu}.$

We use the test function: $f\ = \alpha(r - a)/(r_1 - a)$

For two phase flow, the Poisson equation becomes:

$$-\frac{G_i}{\mu_i} = \nabla^2 w_i\ ; i=1,2$$

where G_i is the pressure drop per unit length in phase i and μ_i is the respective phase viscosity. The boundary conditions on the fluid- solid boundaries are no slip (i.e. $w_i(x, y) = 0)$. For $(x, y) \in \Gamma_i$; $i = 1, 2$, a two-phase system is schematically shown in Figure 1 and 2. With equal velocities and shear stresses at the fluid-fluid interface with equal velocities and shear stresses at the fluid-fluid interface:

$w_1(x, y) = w_2(x, y)$ for $(x, y) \in \Gamma_{12}$ and $\mu_1 \hat{n}_{12}\nabla w_i(x, y) + \mu_2 \hat{n}_{21}\nabla w_2(x, y) = 0$ for $(x, y) \in \Gamma_{12}.$

Figure1: Two phase description.

Matrix

Gas

Water

Figure 2: Model of Pore Channel (Two Phases)

To address this problem in a variational context, the velocities w_1 and w_2 are replaced by test functions f_1 and f_2 containing free parameters that are chosen to minimize a functional. The test functions need not satisfy the governing Poisson equations exactly nor the shear stress boundary condition. They must, however, must satisfy velocity boundary conditions. Under these conditions, and rather weak conditions on continuity, it can be shown that an optimal choice of the test parameters is the one that minimizes the functional

$$I[f_1, f_2] = \frac{1}{2}\int_{R_1} dxdy\{\mu_1\nabla f_1 f_1 - 2G_1 f_1\} + \frac{1}{2}\int_{R_2} dxdy\{\mu_2\nabla f_2.f_2 - 2G_2 f_2\}$$

The choice is optimal because it minimizes the viscous dissipation in the system within the constraints of the actual functional forms deployed for f_1 and f_2 : the absolute minimum in the dissipation
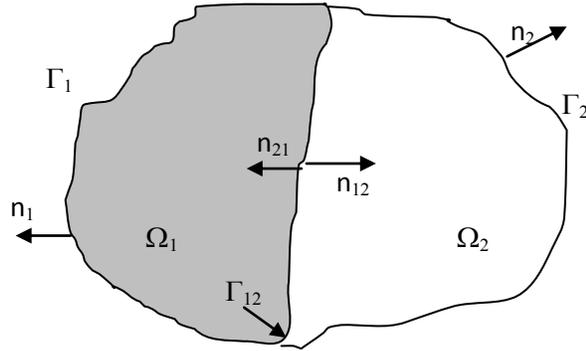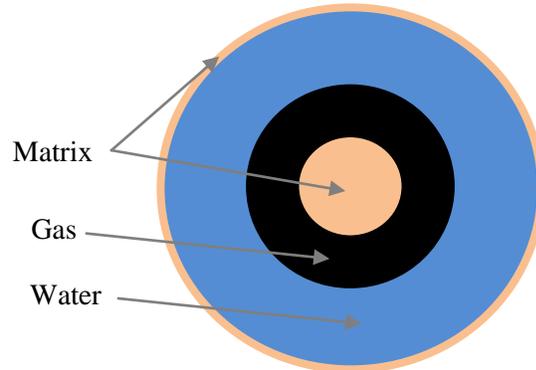
is obtained when $f_i = w_i$. We have, $I[f_1, f_2] \geq -\frac{1}{2}G_1 q_1 - \frac{1}{2}G_2 q_2$, where the phase fluxes are given by $q_i = \int_{R_i} dx\,dy\, w_i$ for $i = 1, 2$ Equality holds if and only if $f_i = w_i$.

III. Results

To validate single phase case, first, we consider a triangular duct (without loss of generality) and asimple test function, f. Test function is chosen such that it satisfies the boundary condition and is given by $f = Cy(y - \beta x)(y - \beta' x')$. We consider an isosceles triangle cross because empirical results are known for this geometry. For isosceles triangle, we get $a = 1/2$ and $\beta = \beta'$. After performing variational analysis for this case, we compute the formula for hydraulic conductance, $g = \frac{\beta^3}{160(3+\beta^2)}$. From lubrication theory, the empirical formula for hydraulic conductance is given by $g_{emp} = 0.6\frac{area^3}{perimeter^2} = \frac{3\beta^3}{320(1+\sqrt{1+\beta^2})^2}$.

(a,b)

(0,0)   (1,0)

$\beta = b/a,\ \beta' = b/(1-a)$, and
$x' = (1-x)$

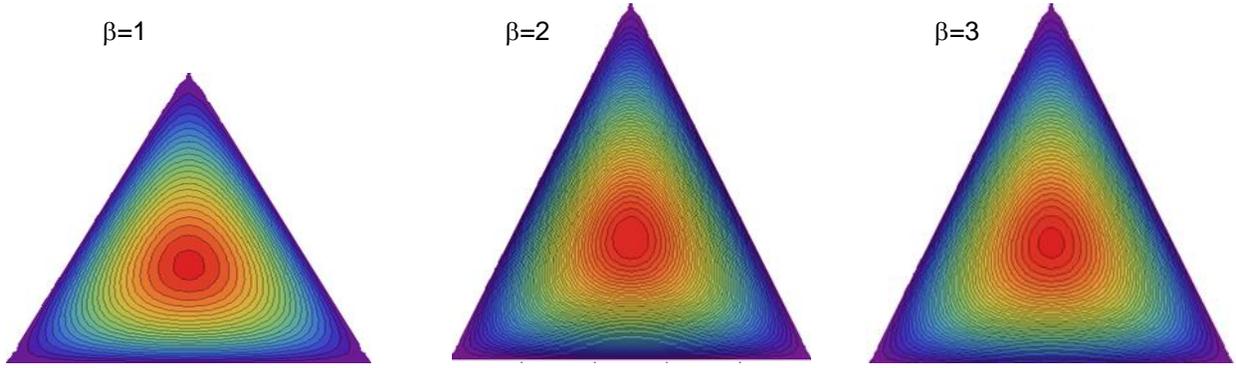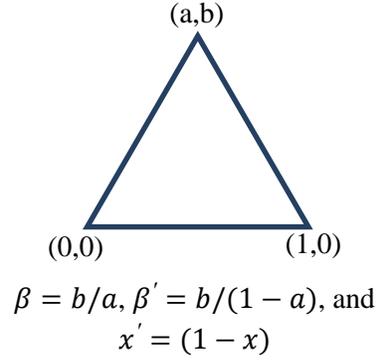β=1   β=2   β=3

Figure 3: Velocity profile through triangular duct (isosceles triangle) for various aspect ratios.

Velocity profile for various aspect ratios is shown in the Figure 3 and the ratio of computed and empirical hydraulic conductance is plotted in Figure 4. For a range of shapes around an equilateral triangle, for which the two formulae coincide, the values are equal to the analytic result.
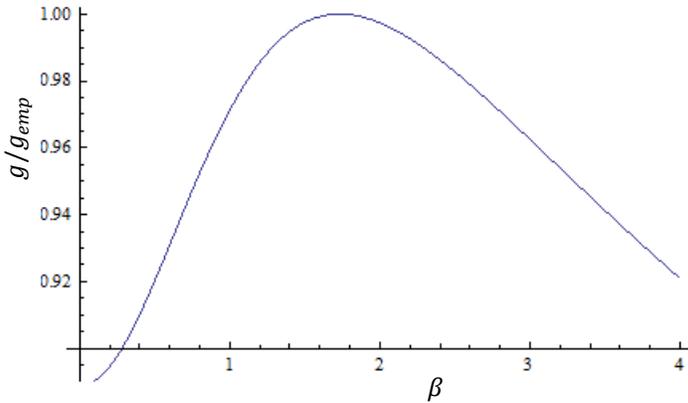

Figure 4: Ratio of *g* to *g*emp for a range of values of β around the equilateral triangle value $\beta = \sqrt{3}$.

We also carried out variational analysis for single phase flow through circular ducts. Analytical solution is available for circular ducts, so this case provides a reliable verification and validation test case for the variational approach. To validate, we considered a simple test functions for f. One parameter (α) test function, that satisfies the boundary condition is given as $f = \alpha(1-r)(r-a)$ and the two

parameters ($\propto$ & β) test function is given as $f = (1-r)[\propto (r-a) + \beta(r-a)^2]$ where , $a < r < 1$. We calculated for the exact solution which is $w = \frac{1}{4}\left[(1-r^2) - \frac{1-a^2}{\ln(1/a)}\ln(1/r)\right]$. Velocity profile through the annulus section as predicted by the variational formulation and relative error in flux is shown in the Figure 3. It is observed that even for very thin core (e.g., a/r_2=0.2), variational approach with both one parameter (<5% error) and two parameters (<2% error) gives very accurate prediction for the flux through the pore.
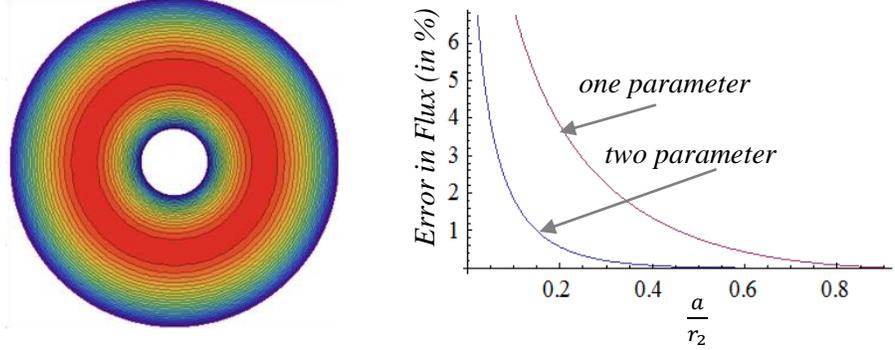

Figure 5: Velocity profile through annulus section as computed from variational principles (Left) with one parameter and error in flux (in %) where *a is the inner radius and r₂ is the outer radius.*

To validate the two phase system, we consider the two phase system as shown in Figure 2. Exact solution for this case is given by:

$w_1 = -\frac{1}{4}\gamma_1(r^2-a^2) + b_1\ln\left(\frac{r}{a}\right)$ and $w_1 = -\frac{1}{4}\gamma_2(r^2-b^2) + b_2\ln\left(\frac{r}{b}\right)$ where

$b_1 = \frac{u_2[\gamma_1(r_1^2-a^2)+\gamma_2(b^2-r_1^2)]+2(\gamma_1\mu_1-\gamma_2\mu_2)\ln\left(\frac{b}{r_1}\right)r_1^2}{4\left[\mu_2\ln\left(\frac{r_1}{a}\right)+\mu_1\ln\left(\frac{b}{r_1}\right)\right]}$ and $b_2 = \frac{u_1[\gamma_1(r_1^2-a^2)+\gamma_2(b^2-r_1^2)]+2(\gamma_1\mu_1-\gamma_2\mu_2)\ln\left(\frac{r_1}{a}\right)r_1^2}{4\left[\mu_2\ln\left(\frac{r_1}{a}\right)+\mu_1\ln\left(\frac{b}{r_1}\right)\right]}$

The exact fluid fluxes are given by $q_1 = -\frac{1}{8}\pi\gamma_1(r_1^2-a^2)^2 + \pi b_1 r_1^2\ln\left(\frac{r_1}{a}\right) - \frac{1}{2}\pi b_1(r_1^2-a^2)$ and $q_2 = -\frac{1}{8}\pi\gamma_2(b^2-r_1^2)^2 + \pi b_2 r_1^2\ln\left(\frac{b}{r_1}\right) - \frac{1}{2}\pi b_2(b^2-r_1^2)$. Approximate solution using variational methods is obtained by using one parameter test functions $f_i, i = 1,2$, which statisfy the boundary conditions in the circular duct. The functions are $f_1 = \alpha(r-a)(r_1-a)$ and $f_2 = \alpha(b-r)(b-r_1)$. The single parameter α appearing is determined by minimizing $I[f_1,f_2]$ and the approximate fluxes are computed by replacing w$_i$ by f$_i$. By minimizing the functional, we got the parameter of the test functions $\alpha = \frac{[(br_1+b^2-2r_1^2)G_2+(2r_1^2-ar_1-a^2)G_1](r_1-a)(b-r_1)}{3[(r_1+a)(b-r_1)\mu_1+(r_1+b)(r_1-a)\mu_2]}$ and the approximate fluid fluxes $q_1 = \frac{1}{3}\pi\alpha(2r_1^2 - ar_1 - a^2)$ and $q_2 = \frac{1}{3}\pi\alpha(r_1 b + b^2 - 2r_1^2)$.

VI. Acknowledgements

V. Bibliography

Abate, J.; Want, P.; & Sepehrmoori, K. (1999). Parallel compositional reservoir simulation on a cluster of PC's. International Journal of High Performance Computing Applications. V. 15 pp 13-21

Babei, M. & King, P. R. (2010). Upscaling Reservoir Simulation using multi-level operator coarsening. XVII International Conference on Water Resources. CMWR 2010. CIMNE, Barcelona 2010.

Chakraborty, S. (2010). Microfluidics and Microfabrication. Springer

Ghomian, Y. (2008). Reservoir Simulation for Coupled CO2 Sequestration and Enhanced Oil Recovery. Dissertation: University of Texas at Austin.

Lopez, X. (2004). Pore Scale Modeling of Non-Newtonian Flow. Dissertation: Imperial College, London.

Sochi, T. (2007). Pore-scale Modeling of Non-Newtonian Flow in Porous Media. Dissertation: Imperial College, London

Sholokhova, Y. (2009). Network flow modeling via Lattice-Boltzmann based channel conductance – prediction of relative permeability in primary drainange. Dissertation: Stony Brook University

Turgay, E. & About-Kassem, J.H. (2001). Basic Applied Reservoir Simulation. SPE Texbook Series, Vol. 7