DOE-ARRA Geologic Sequestration Training and Research 2011 Yearly Review Meeting

Project DE-FE0002407

Title: HIGH FIDELITY COMPUTATIONAL ANALYSIS OF CO2 TRAPPING AT PORE SCALES

University of Texas at El Paso
Presenter: Dr. Vinod Kumar, Dept. of Mechnical Engineering
February 24-26, 2011

Project Participants

- Dr. Vinod Kumar (PI)
- Fan Chen (doctoral student)
- Paul M. Delgado (doctoral student)

Introduction

- Background on the project

  We are developing a multiphase flow conductance model using variational fomulations for generalized pore geometries, integrate the conductance model reservoir simulator, and validated the results against analytical and empirical solutions. We consider test functions to approximate the velocity from the C^2 – continuous inside the pore geometry that satisfies the appropriate boundary conditions.

- Anticipated benefits

  Lack of knowledge of molecular mobility under confinement and molecule-surface interactions between CO2 and natural porous media results in generally unpredictable absorption kinetics and total absorption capacity for injected fluids, and therefore, constitutes barriers to the deployment of this technology. Pore level studies can be used to study these. Additionally, Variational methods provide unique features to study non-Newtonian flows. Non-Newtonian flow physics is important study to the CO2 sequestration and flooding studies.

Project Objectives

- Major Objective
  - Develop computational technique using variational techniques to estimate hydraulic conductance in pores.
  - Construct and Simulate of a multiphase system with regular and irregular geometries.
- Secondary Objectives
  - Apply the Conductance Equation to a Reservoir Simulator.
  - Improve the fidelity of physics based modeling for bettering understanding the kinetics of CO_2 trappings inside porous media.

Project Funding

- Total Project Cost: $288K, 3 Year
- DOE Share: $288K
- Non-DOE Cost Share: $0
- Cost Share Provider: N/A

Highlights of Project to Date

- Hired two doctoral students and graduate a MS student!
- Completed flow conductance derivations and calculations for single and two-phase system.
- Chose the reservoir, installed it on Linux computer, and got started with simple cases

Tasks – Overview

Task No.	Task Description	Task Duration	Task Funding (estimated)
1	Project Management and Planning	12/01/2009 – 11/30/2012	$
2	Construction and Simulation of a Simple, Single Phase Model	12/01/2009 – 11/30/2010	$70K
3	Construction and Simulation of a multiphase system with regular and irregular geometries	09/01/2010 – 11/30/2011	$100K
4	Reservoir simulations	12/01/2009 – 11/30/2011	$50K
5	Apply Conductance Equation to Reservoir Model	06/01/2011 – 11/30/2012	$68K
		Total (with indirect)	$288K

Project Schedule

Task Title	Project Tasks	Budget Period: 1st half						Budget Period: 2nd half					
		Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8	Q9	Q10	Q11	Q12
Program Management	Task 1												
Simple model	Task 2												
External Resources	Task2.1												
Build simple model	Task2.2												
Single phase flow model	Task2.3												
Verification of the Model	Task2.4												
Multiphase system	Task 3												
Build multiphase model	Task3.1												
W/ Complex Geometries	Task3.2												
Verification of the Model	Task3.3												
Reservoir simulations	Task4												
Choose the reservoir	Task4.1												
Lab-Scale System	Taskt4.2												
Conductance derivation	Taks4.3												
Experimental Data	Task4.5												
Coupled Model	Task5												
Code Integration	Task5.1												
Simulations & verification	Taks5.2												

Discussion – Variational method

Variational methods seem a promising way of obtaining approximate analytical expressions for hydraulic conductance of pore elements for input into pore network models

The methods seem to promise better approximations for hydraulic conductance of pore throats partitioned among two or more phases than the traditional free-slip/ no-slip approach

Further validation is required:

E.g. – single-phase phase flow with mixed fs/ns boundaries, compare with finite element solutions

Variational Methods

Most treatments start by considering the one-dimensional case

$$I[f] = \int_a^b dx F\{x, f, f_x\}$$

By considering variations of f, stationary points of I can be determined → Euler-Lagrange equations

E.g. Isoperimetric Problem
(subject to integral constraint)

Variational Methods (cntd)

The solution of ordinary and partial differential equations can be expressed in terms of the minimization of a functional – i.e. differential equation → F

Use test functions f_{test} and select parameters in them to minimize $I(f_{test})$ → approximate solution of differential Equation

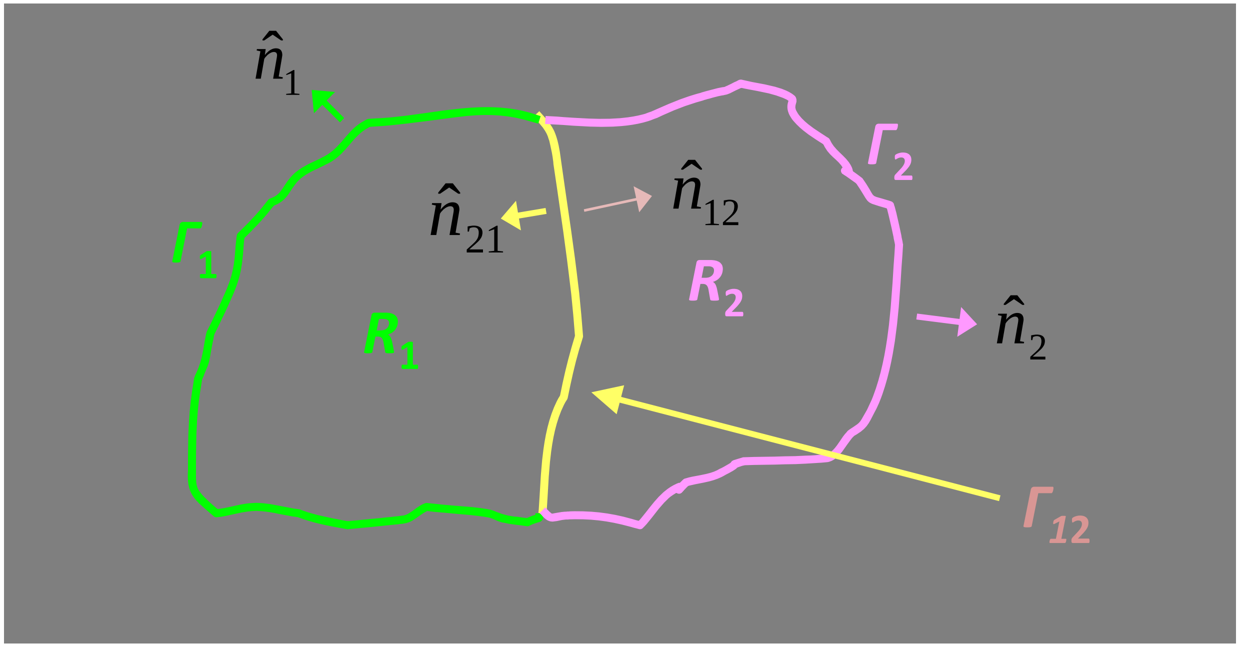
Global minimization using test function over whole domain → approximate solution in analytical form

Local minimization over sub-domains → finite elements

Variational Methods (cntd)

<u>Application to two-phase flow in a straight duct</u>

Let R comprise regions R_1, R_2 containing fluids 1 & 2, viscosities μ_1, μ_2 respectively. Fluid interface Γ_{12}, boundaries of R_1, R_2 with duct wall Γ_1, Γ_2.



Variational Methods (cntd)

The fluid velocities $w_1(x,y)$ & $w_2(x,y)$ satisfy

$$\nabla^2 w_i = -G_i / \mu_i \qquad (x,y) \in R_i$$

BCs $\quad w_i(x,y) = 0 \qquad (x,y) \in \Gamma_i$

$$\left.\begin{aligned} & w_1(x,y) = w_2(x,y) \\ & \mu_1 \hat{n}_{12} . \underline{\nabla} w_1(x,y) + \mu_2 \hat{n}_{21} . \underline{\nabla} w_2(x,y) = 0 \end{aligned}\right\} \quad (x,y) \in \Gamma_{12}$$

Introduce a functional $I[f_1,f_2]$ such that

f_i is any C_2-regular function vanishing on Γ_i

and $f_1 = f_2$ on Γ_{12}

Discussion – Task 2

- Simple Model using Vairational approximation
  - External Resource (Kumar) 100%
  - Build simple model (Kumar, Kavoori, Chen) 100%
  - Single phase flow model (Kumar, Kavoori, Chen) 100%
  - Verification of the model (Kumar, Kavoori, Chen) 100%
- Verified triangular and circular single phase models

Simple Case - Single-phase Flow

Set $G = \mu = 1$ without loss of generality

$$I[f] = \frac{1}{2}\int_R dxdy\,\{\underline{\nabla} f.\underline{\nabla} f - 2f\}$$

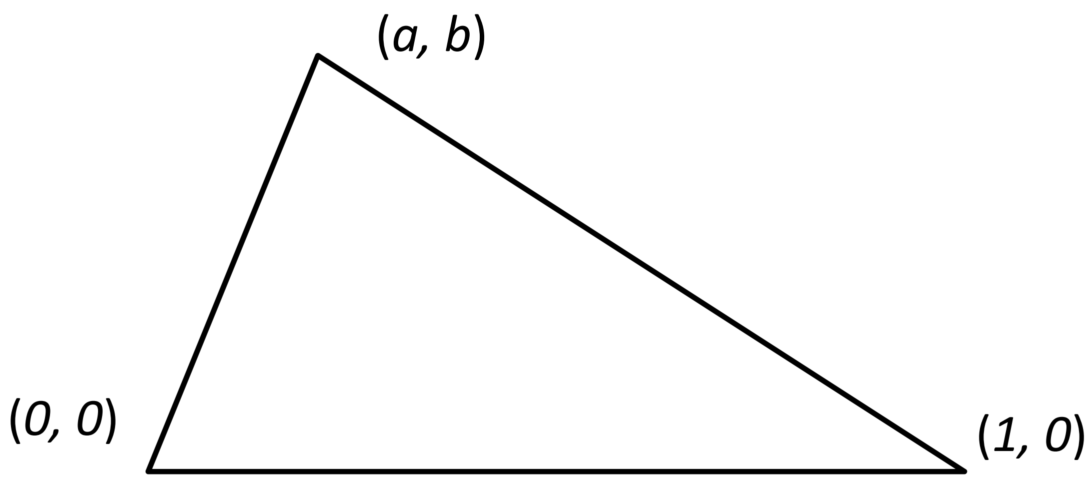
Let $f = \sum_{k=1}^{n} \alpha_k f_{test}^{(k)}$

Define $I_{var} = \min I[f]$

$$I_{var} = -\frac{1}{2} q^{var}$$

$$q^{var} = \int_R dxdy\, f$$

Newtonian Flow in Isosceles Triangular Cross-Section Duct



Analytical Solution

Empirical Hydraulic Conductance

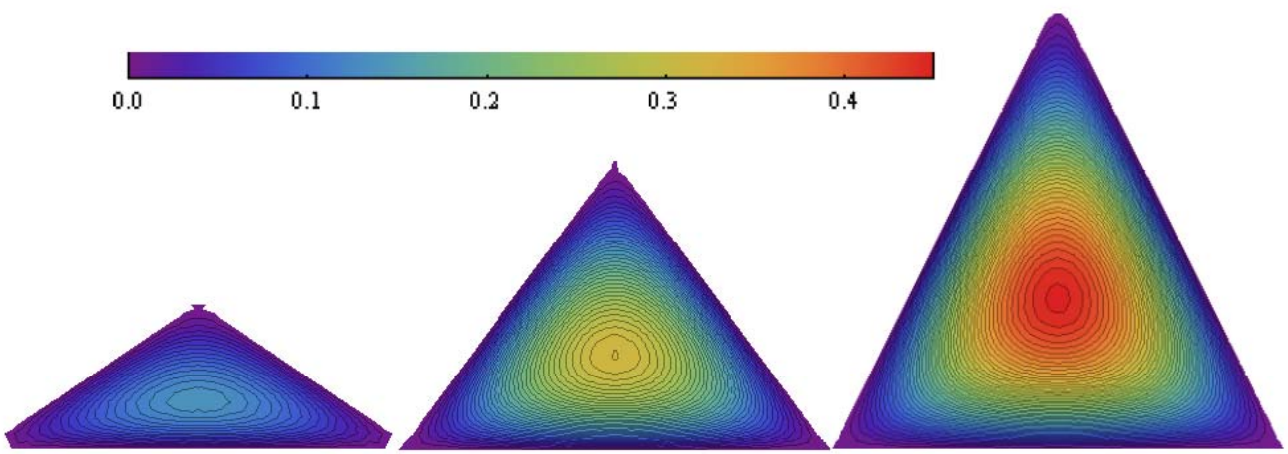
$$g_{emp} = \frac{0.6(area)^3}{(perimeter)^2} = \frac{3\beta^3}{320\left(1+\sqrt{1+\beta^2}\right)^2}$$

Variational Approach

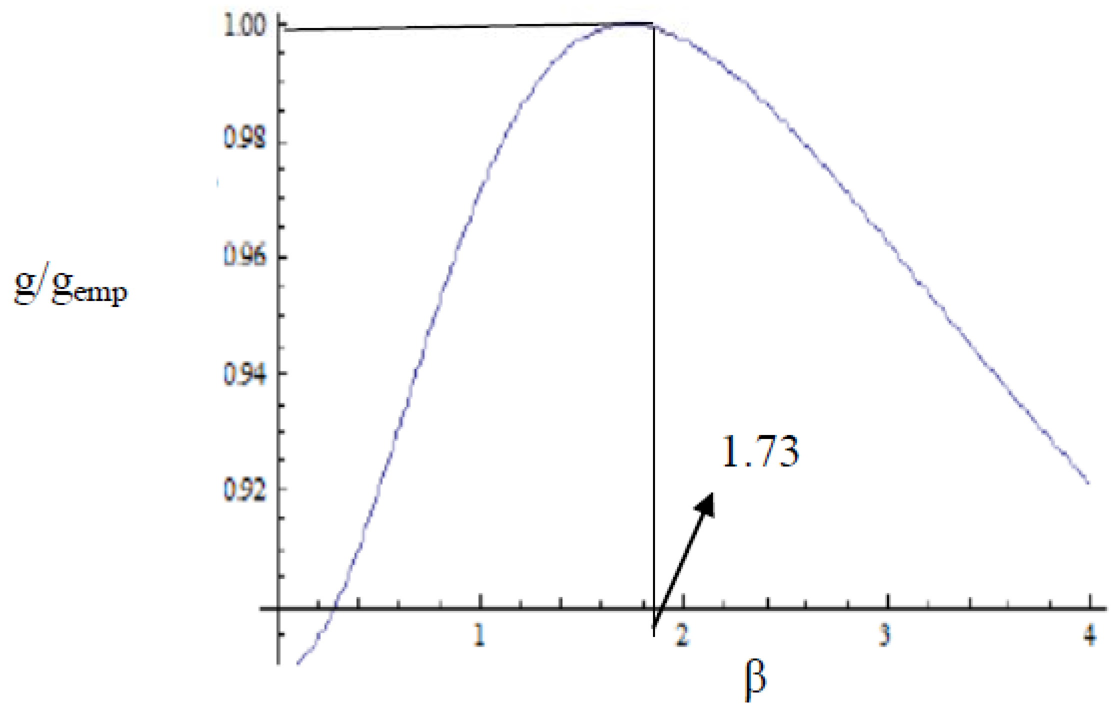
One-parameter test function

$$f = \alpha y(y - \beta x)[y + \beta'(x - 1)]$$

$$where\ \beta = \frac{b}{a}, \beta' = \frac{b}{1-a}$$



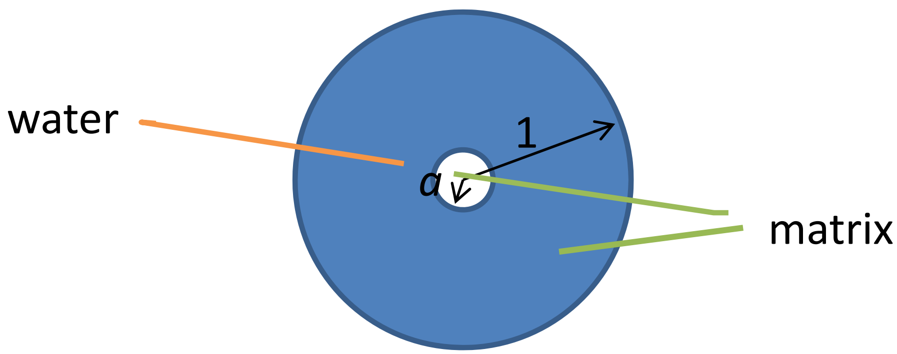
$\beta = 1$ $\beta = 2$ $\beta = 3$



1.00
0.98
0.96
0.94
0.92
g/g_emp
1
2
3
4
β
1.73

Newtonian Flow in Circular Cross-Section Duct

Annular flow: $a < r < 1, \frac{G}{u} = 1$



Analytical Solution

$$w = \frac{1}{4}\left[\left(1 - r^2 - \frac{(1 - a^2)}{\ln\left(\frac{1}{a}\right)}\ln\left(\frac{1}{r}\right)\right)\right]$$

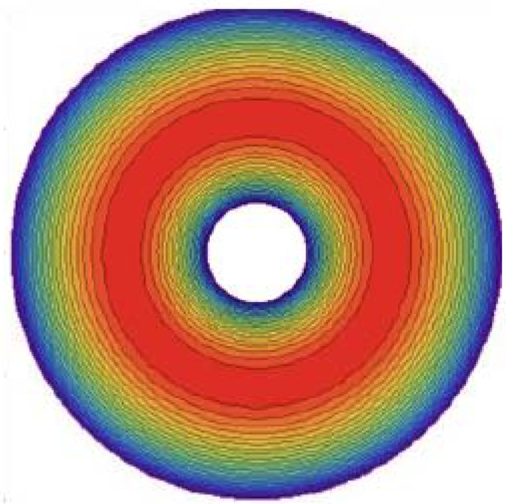
Variational Approach

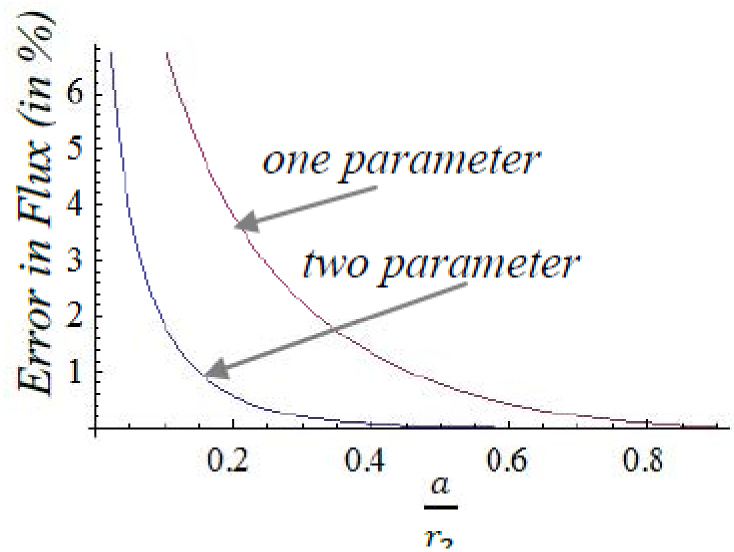
Test function with one parameter α:

$$f = \alpha(1 - r)(r - a)$$

Test function with two parameters α, β:

$$f = (1 - r)[\alpha(r - a) + \beta(r - a)^2]$$





Error in Flux (in %)
one parameter
two parameter
0.2
0.4
0.6
0.8
1
2
3
4
5
6
a
r2

Non-Newtonian Flow in Circular Cross-Section Duct

$$\nabla.(\mu\nabla w) = -\left(-\frac{dp}{dz}\right) = -G$$

where $\mu = k\left|\frac{dw}{dr}\right|^{n-1}$

Considered n = 0.5

Analytical Solution

$$w_1 = \frac{G^2}{4k^2}\left[\left(\frac{r^3}{3} - \frac{4C}{G}r - \frac{4C^2}{G^2}\frac{1}{r}\right) - \left(\frac{a^3}{3} + \frac{4C}{G}a - \frac{4C^2}{G^2}\frac{1}{a}\right)\right]$$

$$where\ r < r_0\ and\ \frac{dw}{dr} > 0$$

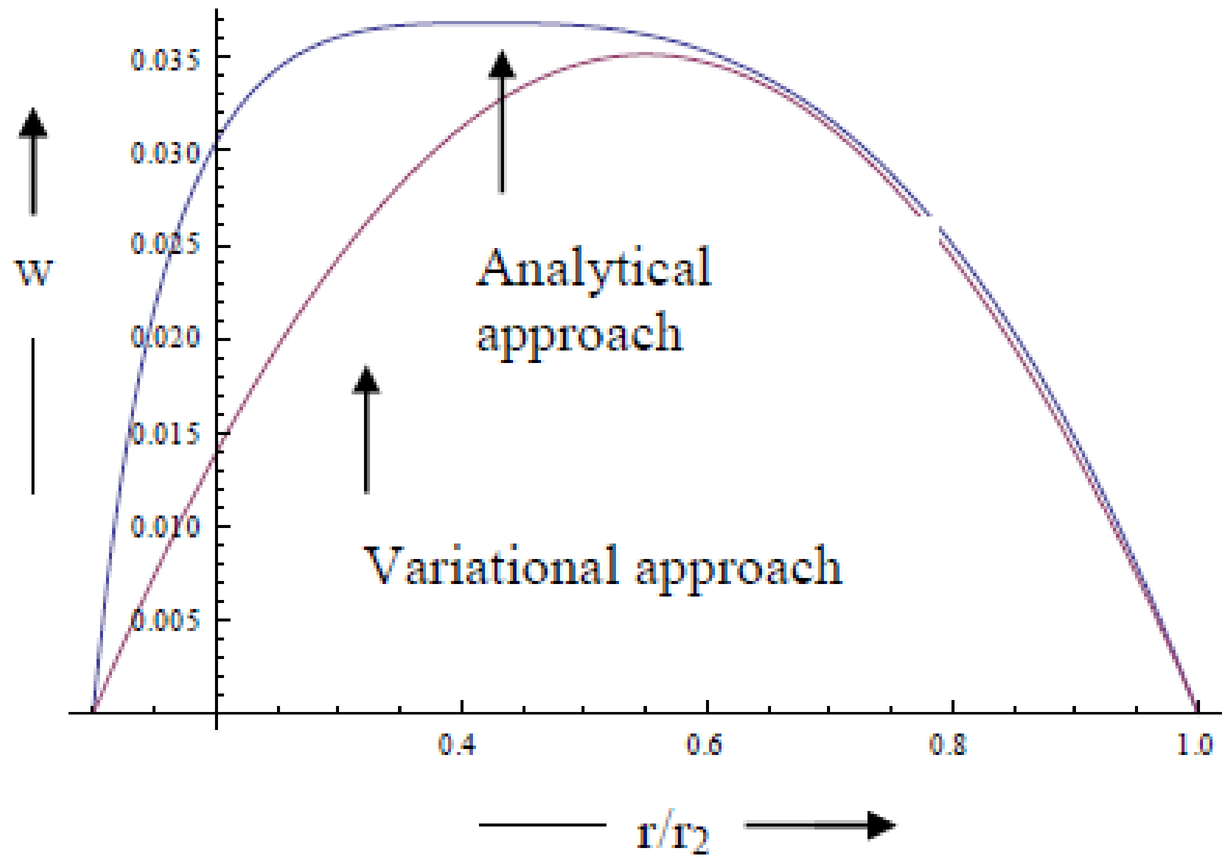
$$w_2 = \frac{G^2}{4k^2}\left[-\left(\frac{r^3}{3} - \frac{4C}{G}r - \frac{4C^2}{G^2}\frac{1}{r}\right) + \left(\frac{r_2^3}{3} + \frac{4C}{G}r_2 - \frac{4C^2}{G^2}\frac{1}{r_2}\right)\right]$$

$$where\ r > r_0\ and\ \frac{dw}{dr} < 0$$

Variational Approach

$$f = c(1-r)(r-a)$$

$$where\ c = \left[\frac{5(1-2a+2a^3-a^4)}{18((1-a)^{5/2}+(1-a)^{5/2}a)}\right]^2$$

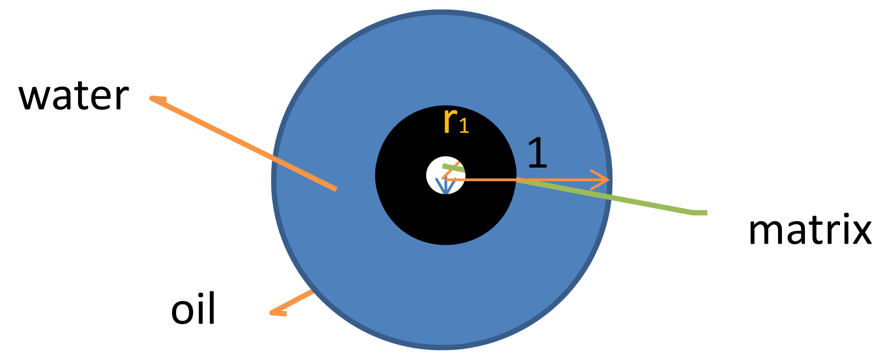

0.035
0.030
0.025
0.020
0.015
0.010
0.005
w
0.4
0.6
0.8
1.0
r/r2
Analytical approach
Variational approach

Discussion – Task 3

- Multiphase System
  - Build multiphase model (Kumar, Chen) 100%
  - W/Complex Geometries (Kumar, Chen) 0%
  - Verification of the model (Kumar, Chen) 50%
- Verified two-phase circular model – 100%

Two-Phase Newtonian Flow in Circular Cross-Section Duct

Phase 1: $a < r < r_1$



Phase 2: $r_1 < r < b$

$$\gamma_i = \frac{G_i}{\mu_i}, \qquad i = 1,2$$

Analytical Solution

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

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

With

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

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

Fluxes:

$$q_1 = -\frac{1}{8}\pi\gamma_1(r_1^2 - a^2)^2 + \pi b_1 r_1^2 \ln\left(\frac{r_1}{a}\right) - \frac{1}{2}\pi b_1(r_1^2 - a^2)$$

$$q_2 = -\frac{1}{8}\pi\gamma_2(b^2 - r_1^2)^2 + \pi b_2 r_1^2 \ln\left(\frac{b}{r_1}\right) - \frac{1}{2}\pi b_2(b^2 - r_1^2)$$

Variational Approach

One parameter test functions

$$f_1 = \frac{\alpha(r-a)}{r_1 - a}$$

$$f_2 = \frac{\alpha(b-r)}{b - r_1}$$

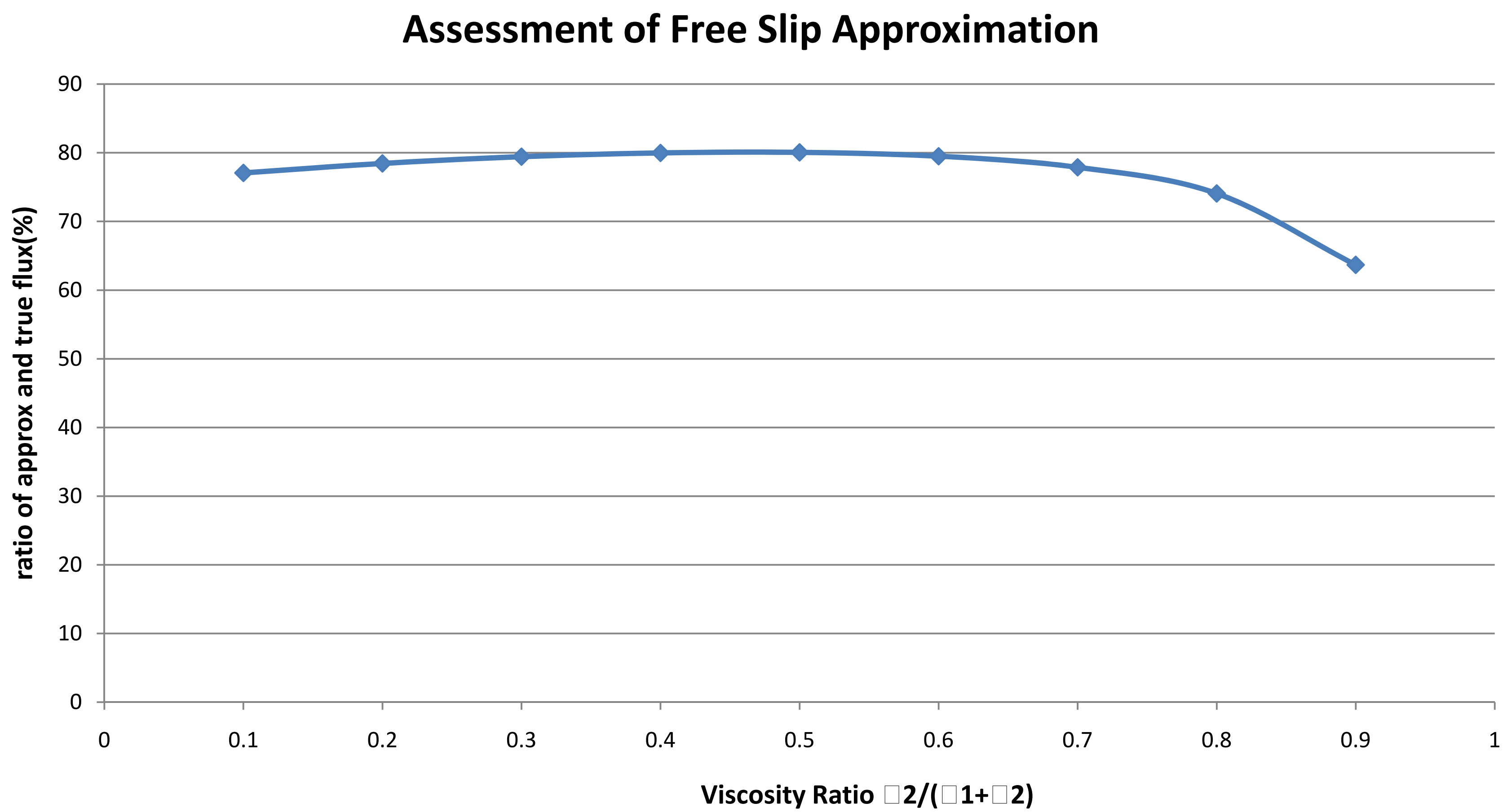
With $\alpha = \frac{[(br_1+b^2-2r_1^2)G_2+(2r_1^2-ar_1-a^2)G_1](r_1-a)(b-r_1)}{3[(r_1+a)(b-r_1)\mu_1+(r_1+b)(r_1-a)\mu_2]}$

The test functions satisfy $f_i = 0$ on $\Gamma_i, i = 1,2$,
$f_1 = f_2$ on Γ_{12}

Flux

$$q_1^{(var)} = \frac{1}{3}\pi\alpha(2r_1^2 - ar_1 - a^2)$$

$$q_2^{(var)} = \frac{1}{3}\pi\alpha(r_1 b + b^2 - 2r_1^2)$$


Assessment of Free Slip Approximation
ratio of approx and true flux(%)
Viscosity Ratio □2/(□1+□2)
90
80
70
60
50
40
30
20
10
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Discussion – Task 4

- Reservoir Simulations
  - Choose the reservoir (Kumar) 100%
  - Lab-Scale System (Kumar) 50%
  - Conductance Derivation (Kumar) 100%
- Major accomplishment(s)
  - Installed MASTER 3.0 software
  - Executed five example simulations included with software
  - Currently editing input files for CO_2 sequestration simulation.
- Major issues/problems (if applicable)
  - Non user friendly input file interface.
  - Complexity of documentation files.

Project Milestones

(Include HQ and project milestones)

Milestone	Planned Completion Date	Actual Completion Date
Milestone 1.1: Data collection from external resources and formulation for simple model	4/1/2010	4/1/2010
Milestone 1.2: Development of Single Phase Model and Getting started with a reservoir model	8/1/2010	8/1/2010
Milestone 1.3: Completion of Simple Model, Run reservoir model on a lab-scale system	12/1/2010	12/1/2010

Project Milestones

Task Title	Project Tasks	Budget Period: 1st half						Budget Period: 2nd half					
		Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8	Q9	Q10	Q11	Q12
Program Management	Task 1												
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Verification of the Model	Task2.4												
Multiphase system	Task 3												
Build multiphase model	Task3.1												
W/ Complex Geometries	Task3.2												
Verification of the Model	Task3.3												
Reservoir simulations	Task4												
Choose the reservoir	Task4.1												
Lab-Scale System	Taskt4.2												
Conductance derivation	Taks4.3												
Experimental Data	Task4.5												
Coupled Model	Task5												
Code Integration	Task5.1												
Simulations & verification	Taks5.2												

Anticipated Efforts for the Coming Year

- Construction of multiphase flow through regular and complex pore geometries.
- Verification and validation of results for single & multi - phase flows with existing lab test data.
- Construction of pore-network model for regularized and irregular (e.g., through CT-scanned images) geometries .

PI Contact Information

- If you have any questions or would be interested in collaboration please contact

vkumar@utep.edu (email) or

915-717-6075 (phone)