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COMSOL Simulations of Density Fingering Instability in Channel

Anoop Kumar[1] Ashok Kumar[2]*

[1,2] Net Qualified

Abstract – Density fingering instability obtained when a more dense fluid lie on the less dense fluid and it is very fundamental importance in CO_2 −sequestration. In literature, various model are available for CO_2 −sequestration. process. Comparison and validity of various model were discussed. In this work, we perform the simulation in channel by taking unsteady Stoke's equation with forcing term. COMSOL multiphysics software is used to simulate the problem. Our results suggest that for low Atwood number, vertical centreline symmetry is obtained. Also, we show when Atwood number high, due to dominance of inertial force on viscous force, very chaotic instability is obtained.

Keywords: COMSOL, Unsteady Stoke's Equation, Atwood Number, Vorticity.

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1. INTRODUCTION

Various type of instability occures in nature depends on difference in various properties. Density fingering (DF) instability is one of them due to difference in density [1]. Due to more density of upper fluid, there is finger-like instability developed at the fluid-fluid interface and hence called as density fingering instability. Fluids can be miscible or immiscible or partial miscible in nature. In this work, we assumed fluids are miscible in nature. DF has various applications in literature such as enhanced oil recovery, CO_2 sequestration, groundwater contamination etc [2, 3, 4]. CO_2-sequestration process in very important, in which CO_2 is stored in the underground [4].

Density-driven instability with Navier-Stoke's, unsteady Stoke's, Darcy's law is studied by various authors [5, 6, 7, 8]. Sahu studied the two-fluid flow in horizontal channel and vertical channel, which is governed by Navier-Stokes equation [6, 7]. DF governed by Darcy's law with gravity term in porous media is studied by Riaz *et al* [4]. Thus, various literature exists and work is going on depending on governing equation. Linear stability analysis as well as non-linear simulations are studied early with different-different method. In this paper, we studied using unsteady Stokes equation. In section 2, mathematical modelling is discussed of the problem. In section 3, use of COMSOL to solve the problem as well as implementation of initial conditions and boundary conditions are discussed. Then, results of the simulations are studied in section 4. Our finding suggest that symmetric pattern are obtained for low atwood number.

2. MATHEMATICAL MODELING

A fluid of density ρ_{upp} lie on the fluid having density ρ_{low} in a two-dimensional rectangle medium. Domain is $(x,y) \in \left[-\frac{L_x}{2},\frac{L_x}{2}\right] \times \left[-\frac{L_y}{2},\frac{L_y}{2}\right]$ and fluid-fluid interface is at *x=0* (see figure [1]). Both the fluids are assumed of same viscosity μ, incompressible and miscible in nature. Since, fluids are miscible so concentration of solute in solvent (*c*) plays an important role. By non-dimensionlisation, without loss of generality concentration of upper and lower fluid are assumed 1 and 0, respectively. Besides, diffusion between the fluids are assumed isotropic and constant in nature.

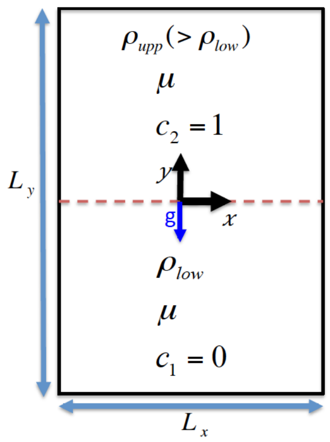

Figure 1. Schematic diagram of 2D flow where dashed line show the unperturbed fluid-fluid interface

To describe the problem, hydrodynamic part for fluid velocity has to be taken and convection-diffusion equation to be taken for conservation of dilute species. In hydrodynamics part, conservation of mass is governed by divergence-free velocity field and unsteady Stoke's equation is taken for conservation of momentum. Thus, mathematically the governing equations are [5, 6, 7, 8] as follow:

$$\nabla\cdot\vec{u}=0 \qquad (1)$$

$$\rho\frac{\partial\vec{u}}{\partial t}=-\nabla\cdot\left[-p\vec{I}+\mu\left(\nabla\vec{u}+(\nabla\vec{u})^{t}\right)\right]+\rho(c)\vec{g} \qquad (2)$$

$$\frac{\partial c}{\partial t}+\vec{u}\cdot\nabla c=D\nabla^2 c \qquad (3)$$

where $\vec{u}=(u,v)$ is the two-dimensional velocity vector, $\vec{I}$ is the identity vector and superscript 't' stands for the transpose. In addition, p is the hydrodynamics pressure, and g is the gravitational acceleration constant ($9.8\ m^2/s$) which is downward and acting on the center. Density(ρ) related to concentration by $\rho(c)=\rho_{low}+\beta c$ where $\beta=\frac{\rho_{upp}-\rho_{low}}{c_1-c_0}$.

3. USE OF COMSOL MULTIPHYSICS

Creeping flow (spf) and transport of dilute species (tds) of COMSOL multiphysics (trial vesion) 5.2a are used for the simulations. COMSOL "spf"-model take care of hydrodynamic part, both incompressible continuity equation and unsteady Stoke's equation with forcing term. COMSOL "tds" model has the convection-diffusion equation where velocity is coupled through spf-model velocity field.

Appropriate initial conditions are described by

$$c(x,y,0)=\begin{cases}1, & if\ y>0\\ 0, & if\ y<0\end{cases} \qquad (4)$$

$$p(x,y,0)=0 \qquad (5)$$

$$\vec{u}(x,y,0)=0 \qquad (6)$$

Discontinuity in concentration at $y = 0$ is removed by smoothing the curve in COMSOL. Initially transition zone between the two fluids is taken *0.001 m*.

Suitable boundary condition for our problem are described in figure 2. At vertical walls, no slip and no flux boundary conditions are given. At upper wall, dirichlet boundary conditions $c = 1$ and $\vec{u}=(0,0)$ are given. Lower boundary conditions for pressure was tricky and implement in comsol as shown in figure 2 for consistent solution.

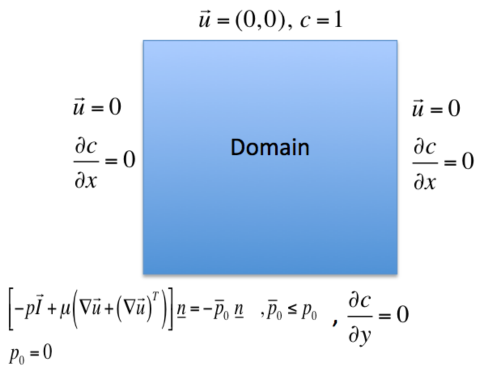

Figure 2. Schematic of boundary conditions

Atwood number (A) is the non-dimesionlised number which is defined as

$$A=\frac{\rho_{upp}-\rho_{low}}{\rho_{upp}+\rho_{low}} \qquad (7)$$

List of parameters

Parameter	Symbol	Value and unit
Width of domain	L_x	0.02, 0.1 m
Height of domain	L_y	0.08, 0.1 m
Viscosity of the fluids	μ	1 mPa s
Diffusion coefficient	D	$10^{-7}\ m^2/s$
Density of Upper fluid	ρ_{upp}	1083.33, 3000 kg/m^3
Density of Lower fluid	ρ_{low}	1000 kg/m^3

Atwood number effect on the instability is studied in our results. In our study, we discussed the instability when *A* is 0.04 and 0.5. Meshing is important to study any physical problem numerically. In this work, extra fine mapped mesh is used for low Atwood number 0.04 and extra fine mapped mesh with boundary layer meshing of COMSOL is used for *A = 0.5*, to discritised the domain.

4. RESULTS AND CONCLUSIONS

First, we simulate the problem for *A = 0.04*. In that case, L_x is taken 0.02 m and L_y 0.08 m. Extra fine mapped mesh is sufficient to study this problem. Grid test is also performed and found that the characteristics of instability are consistent by taking more refine mesh. For *A* > 0 , density fingering occurs as shown in figure 3 for A = 0.04. In the early time, diffusion is occures between the fluids and then due to non-linear convection instability developed (see figure 3). In addition, Interestingly vertical centreline symmetry is obtained.

Now, we perform the simulation when $\rho_{upp} = 3000\ kg/m^3$ and $\rho_{low} = 1000\ kg/m^3$, hence *A = 0.5*. Since, the density difference large here as compare to previous case, more instability is occurred here and more chaotic instability is obtained. Hence, to capture and study the instability phenomena, here L_x is taken 0.1 m and L_y is 0.1 m, large enough. Also, more refine mesh is used near the boundary for getting accurate results. So, extra fine mapped mesh with addition of boundary layer mesh is used to simulate the problem. In this case, density difference is very high, so vorticity effect dominates due to dominance of inertial force on viscous force. Also, in this case, centreline symmetry is not follow as previous case.

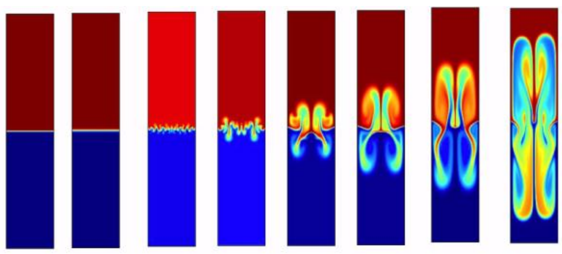

Figure 3. Spatio-temporal evolution of solute concentration at time t = 0, 0.5, 1.1, 1.3, 1.7, 2, 2.4, 3 seconds for *A* = 0.04.

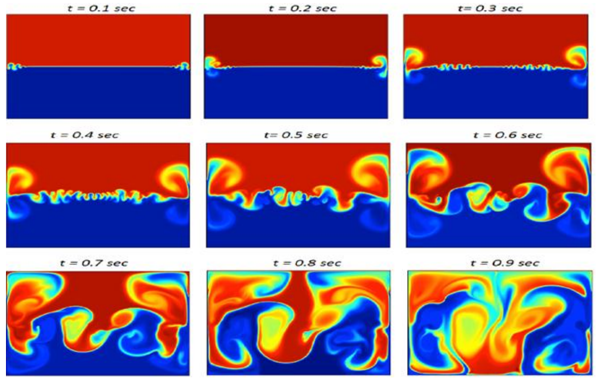

Figure 4. Spatio-temporal evolution of solute concentration at time *t* = 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9 seconds for *A=0.5*.

5. CONCLUSION

Our comsol model is able to capture the density fingering instability. Also, when less dense fluid lie above on more dense fluid, no instability is obtained (not shown in the paper). We simulate the problem for Atwood number 0.04 and 0.5. Our instability patterns for *A = 0.04* and *A = 0.5,* comparable with result obtained by K. Kadau [9]. Also, we shows symmetric pattern are obtained for *A* = 0.04. Simulate the density fingering instability with fully Navier-Stoke's equation is one of the future aspect.

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Corresponding Author

Ashok Kumar*

Net Qualified