Radial Fingering Instability induced by a Precipitation Reaction

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Finger instability caused by the reaction is observed in the precipitation reaction. In this study, the instability was numerically calculated with radial geometry. The mobility change due to precipitation was analyzed, and the results were consistent with the experimental results.

1. Introduction

When two chemical species react to produce a solid product, the reaction is termed as a precipitation reaction and the solid product is called precipitate. If we consider the displacement of one specie by the other, the precipitates formed during the precipitation reaction decrease the mobility in the direction of the flow. This hinders the stable displacement of the reactants, resulting in fingering instability. This fingering instability is important in context of CO_2 sequestration[1]. Consequently, it is important to understand the instability induced by the precipitation reaction.

The fingers produced also depend on the properties of the reactants[1]. Nagatsu *et al.*[1], experimentally reported that depending upon the diffusion coefficient of the two reactants, the fingering patterns and the distribution of the precipitates is different. In their study, the experiments are performed in a radial Hele Shaw cell, in which one reactant radially displaces the other. Further, the experimental study is supported by numerical simulations performed by considering a rectilinear displacement of the two reactants. It must be noted that the two kinds of displacements, viz., radial and rectilinear, have fundamental differences[2] which affect the fingering dynamics too. Consequently, we perform radial simulations to gain insight into the precipitation reaction.

2. Mathematical formulation

We consider the two reactants to be Newtonian, incompressible and miscible in nature. In reference to CO_2 sequestration, we consider the flow through porous media. The dimensionless governing equations are

$$\nabla \cdot \vec{u} = 0, \tag{1}$$

$$\nabla p = -\frac{1}{\kappa(c)}\vec{u}, \tag{2}$$

$$\partial_t a + \vec{u}\cdot\nabla a = \frac{1}{Pe_A}\nabla^2 a - Daab, \tag{3}$$

$$\partial_t b + \vec{u}\cdot\nabla b = \frac{1}{Pe_B}\nabla^2 b - Daab, \tag{4}$$

$$\partial_t c + \vec{u}\cdot\nabla c = \frac{1}{Pe_C}\nabla^2 c + Daab, \tag{5}$$

$$\kappa(c) = e^{-2R_k c}. \tag{6}$$

where equation (6) describes the change in permeability due to chemical reaction. Here, *A* and *B* are the reactants while *C* denotes the precipitate formed on reaction. $Pe_i = Q/D_i$ is the ratio of the flow rate per unit depth to the diffusion coefficient D_i of specie *i*, *i* = *A, B, C*. We perform non linear simulations using a hybrid numerical scheme based on compact finite difference and pseudo-spectral method[2,3].

3. Results and Discussion

Variation of Pe_A, Pe_B helps to compare with the experimental results of Nagatsu et al.[1] Case α in Nagatsu et al.[1] , corresponds to the displacing reactant with a larger diffusion coefficient than the displaced reactant, while case β corresponds to the opposite case. Hence, for our numerical simulations, $Pe_A < Pe_B$ is the case α and $Pe_A > Pe_B$ is the case β.

In Fig. 1 and Fig. 2, we compare the fingering dynamics for the case α and case β as obtained from the numerical simulations. Clearly, longer fingers are evident in case α in comparison to case β, in accordance with the experimental results of Nagatsu *et al.*[1] Another agreement with the experiments is visible in terms of the distribution of the precipitates which is uniform in case α, while the precipitates are accumulated in case β, interpreted in terms of the maximum concentration of *C*.

(a). (b)

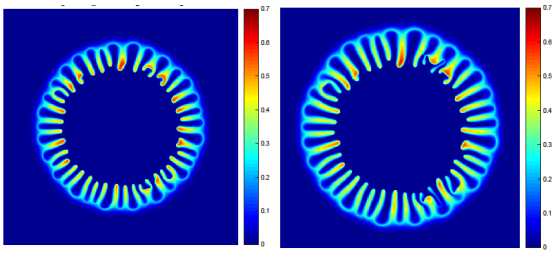

Fig. 1 Density plot of the concentration of product *C* at time (a) t=0.75, (b) t=1 for Case α*: Da=10, R_k=3, Pe_A=200, Pe_B=800, Pe_C=10,000.*

(a). (b)

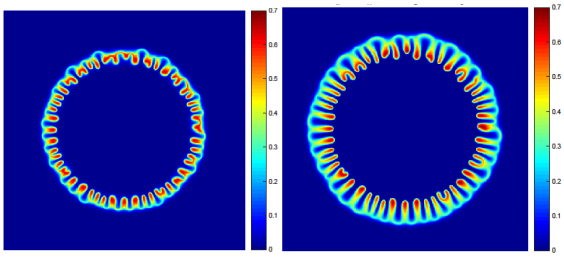

Fig. 2 Density plot of the concentration of product *C* at time (a) t=0.75, (b) t=1 for Case β*: Da=10, R_k=3, Pe_A=800, Pe_B=200, Pe_C=10,000.*

4. Conclusion

Non linear simulations of the fingering induced by precipitation reaction are performed using hybrid numerical method based on compact finite difference and pseudo-spectral method. The results are in good comparison with the existing experimental study.

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