Numerical and Experimental Investigation of Natural Convection Flow of CO_2 in Aqueous

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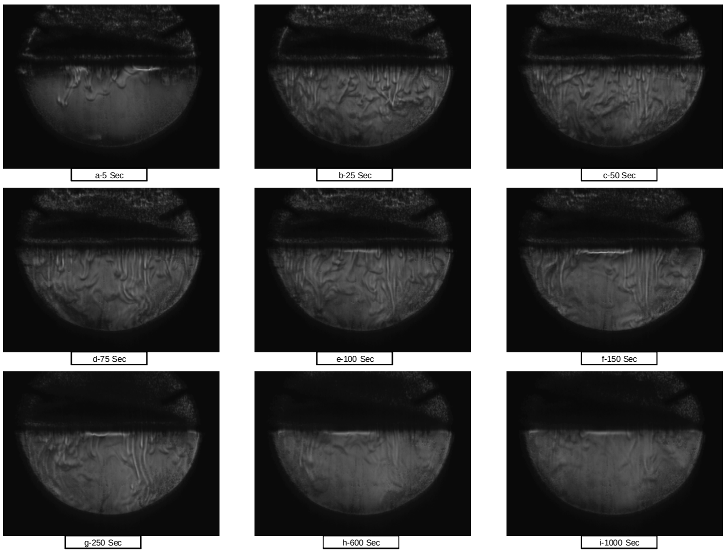
Introduction: Optimal storage of carbon dioxide (CO_2) in aquifers requires dissolution in the aqueous phase.

Experimental Results:

A set of experiments has been done to visualize ($\partial_y c$) the induced convection currents when carbon dioxide is brought above a layer of liquid water, (p=64 bar bar,T=313 K).



Computational Methods:

a) Conventional Formulation:

we consider a 2D cross-section of a cylindrical cell. For the liquid phase, we apply the creeping flow equation and the transport of diluted species in term of pressure, velocity and concentration. At the interface a domain probe and distributed ODE are implemented .

b) Streamline Formulation:

Equivalently We define the stream function and the vorticity as follows :

$$v = \frac{\partial \psi}{\partial y},\ u = -\frac{\partial \psi}{\partial x} \quad (1) \qquad \omega = \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \quad (2)$$

Governing Equations:

$$\nabla^2 \psi = -\omega \quad (3) \qquad \nabla^2 \omega = -Gr\frac{\partial c}{\partial x} \quad (4)$$

$$\frac{\partial c}{\partial t} + \mathbf{v}\ .\ \mathbf{grad}\ c = D\Delta c \quad (5)$$

where ψ is stream function and ω is vorticity. u and v are velocities in x &y driections.

Results: The numerical result is shown in Fig. 1 (22286 elements) and Fig.2 (11566 elements).

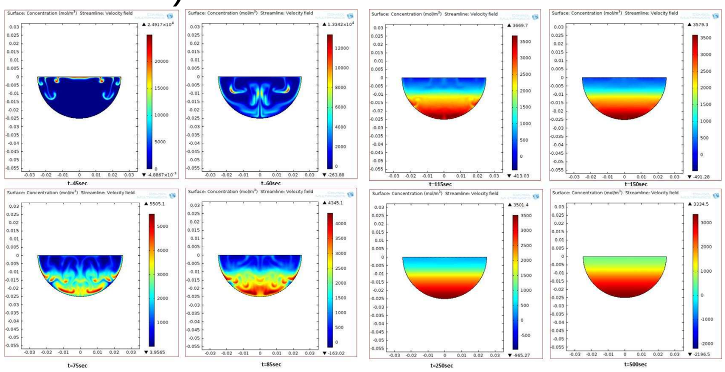


Figure 1 shows a numerical simulation for experimental conditions in the conventional formulation.

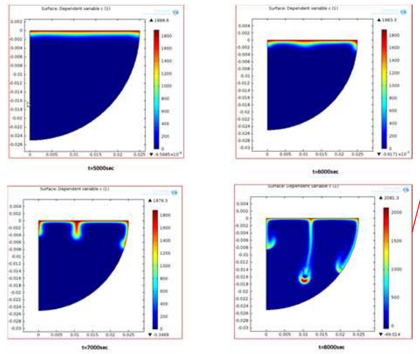


Figure 2 shows a numerical simulation for the experimental conditions in the stream function formulation.

Conclusions:

In principle it is possible to simulate natural convection both with the conventional and the stream function formulation. Both the simulations and the experiment show the existence of a region of high concentration gradient near the gas-liquid interface. However, in the simulation the onset of instabilities occurs later in the experiments.

Denser grid simulations are required for more meaningful comparisons.

References:

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2. Farajzadeh, R.; Zitha P.L.J. and Bruining, J. Enhanced mass transfer of CO2 into water: experiment and modeling. Ind. Eng. Chem. Res., 48 (9), pp. 4542-4552. A.A. (2009)