

Simulation of Gravitational Instability During CO₂ Absorption in a NaHCO₃/Na₂CO₃ Solution

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Abstract

Introduction:

This work deals with the modeling and the numerical simulation of the carbon dioxide (CO₂) absorption, coupled with a chemical reaction, in an initially quiescent aqueous solution of sodium carbonate (Na₂CO₃) and bicarbonate (NaHCO₃), inside a Hele-Shaw cell. In our Hele-Shaw cell, the liquid fills partially the gap between two parallel transparent Plexiglas plates. CO₂ is forced to flow above the liquid in the cell and, therefore, it is absorbed in the liquid. It is observed experimentally, by interferometry, that this absorption, initially driven by diffusion and reaction, leads to the apparition of a gravitational instability, as shown in Figure 1. Assuming that this instability is triggered by a Rayleigh-Taylor mechanism, a two-dimensional model, coupling diffusion, chemical reaction and free convection, is proposed to simulate the development of the instability.

Use of COMSOL Multiphysics®:

To simulate this phenomenon, two user-defined sets of equations are implemented in General Form using the PDE interface on a two-dimensional domain representing the liquid phase in the Hele-Shaw cell.

In the investigated pH range, the reaction in the liquid phase can be written according to this global reaction $\text{CO}_2 + \text{Na}_2\text{CO}_3 + \text{H}_2\text{O} \rightarrow 2\text{NaHCO}_3$. Assuming that the diffusive transports can be modeled by Fick's law, three mass transport-reaction equations (first set) are written.

The flow modeling, aiming at describing the actual three-dimensional flow in the Hele-Shaw cell using a two-dimensional approach, requires averaging the flow along the gap between the two plates of the cell. The Navier-Stokes-Darcy approach is used, assuming a parabolic Poiseuille like profile of the velocity across the gap. It is assumed that the flow is incompressible and the Boussinesq approximation is implied, leading modified momentum transport equations (second set), in which the body force is related to the density variation induced by the concentration variations.

Results:

It is observed that the simulation succeeds to reproduce qualitatively the time evolution of the liquid density variation field in the cell observed experimentally during the onset of the instability and after. The instability starts by the formation of several plumes, between 1 and 2

mm below the interface. These plumes correspond actually to liquid flowing downward, conveying concentrated liquid to the bottom of the cell, while liquid is flowing upward between the plumes. The initial plumes tend to merge to become larger with time.

Conclusion:

In this work, a two-dimensional model is proposed to simulate the Rayleigh-Taylor instability which has been observed in device Hele-Shaw cell when CO₂ is absorbed in an aqueous solution of Na₂CO₃ and NaHCO₃. It is observed that the simulations reproduce rather well the density variation pattern triggering the instability and that the simulated instability dynamics agree qualitatively with the experimental observation. It is well known that such a good agreement between numerical results and experimental results regarding hydrodynamics instability is very difficult to obtain. Therefore, this work highlights the high potential of COMSOL Multiphysics® for flow simulation.

Figures used in the abstract

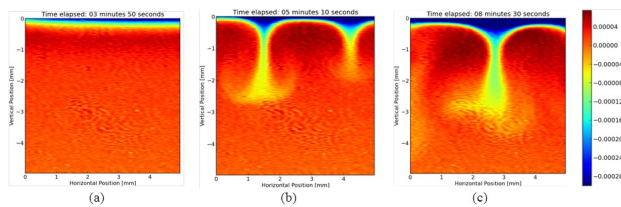


Figure 1: Instability development observed by visualizing experimentally the liquid density variation.

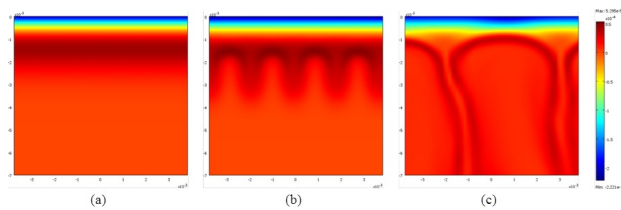


Figure 2: Instability development observed by representing the density variation field simulated with COMSOL Multiphysics®.