

Convective deformation of $A + B \rightarrow C$ reaction fronts

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I. INTRODUCTION

Density changes across a chemical front can lead to hydrodynamical flows that deform the concentration fields in space and time. We analyze such buoyancy-driven flows around an $A + B \rightarrow C$ front in a covered horizontal solution layer. We show theoretically that the dynamics in presence of convection can in that case be predicted solely on the basis of the knowledge of the one-dimensional reaction-diffusion density profile across the front.

II. REACTION-DIFFUSION SYSTEM

When two miscible solutions each containing one reactant of a simple bimolecular reaction $A + B \rightarrow C$ are put into contact, a reaction-diffusion front can develop. Due to the coupling between reaction and diffusion processes, a localized reaction zone extends in time around the initial position of contact between the two solutions. The reaction front is here defined as the location where the production rate of the product C is maximum. The scalings of the propagation of this reaction-diffusion front have been thoroughly studied in the past [1]. Theoretical studies on the diffusion-limited problem have shown that, for long times, the front position scales as a square root of time and that, for equal diffusion coefficients and initial concentrations, the reaction front is stationary i.e. remains at the initial location of contact [1]. Those theoretical works are in good agreement with convection-free experimental studies performed in gels [2].

III. REACTION-DIFFUSION-CONVECTION PATTERNS

However, experiments in horizontal solutions contained between two plates yield very different results to their gel counterparts even with a very narrow gap width. This is supposed to be due to buoyancy-driven convection. As an example, experimental results by Shi and

Eckert [3] are in agreement with the front position scaling of $t^{1/2}$ but the experimental fronts travel much faster than what the standard reaction-diffusion model predicts even for very thin solution layers. Actually, buoyancy effects are operative and induce convection currents speeding up the front.

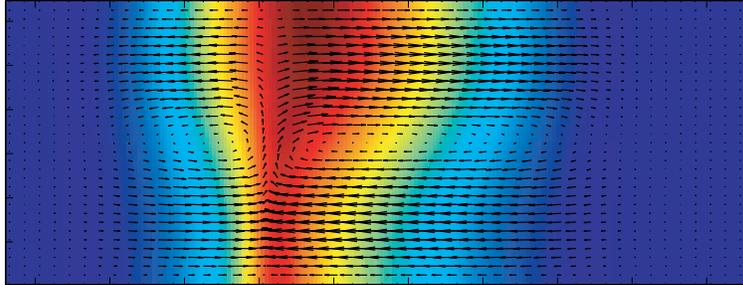


FIG. 1: Numerical simulation of buoyancy-driven convection around a reaction front where the simple $A + B \rightarrow C$ reaction takes place between two solutions containing each of the reactant separately. The arrows show the velocity of the flow superimposed on the concentration field of the product C ranging from its maximum value in red to its minimum one in blue.

In this framework, we have performed theoretical analysis to understand how buoyancy-driven convection affects the problem and modifies the reaction-diffusion dynamics [4]. By numerically integrating the two-dimensional incompressible Stokes equation coupled to reaction-diffusion-convection equations for the concentration of the three chemical species A, B and C , we find that convection not only deforms the reaction front in the layer (Fig.1) but also drastically alters its propagation. Fortunately, a close inspection of the observed dynamics as a function of the parameters of the problem which are the Rayleigh numbers of each chemical species R_a, R_b and R_c shows that the reaction-diffusion-convection dynamics can be fully predicted solely on the basis of the reaction-diffusion density profile across the front.

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