Contribution ID: **590** Type: **Oral Presentation**

Dynamics of $A + B \rightarrow C$ chemical reaction fronts in finite radial geometry

Monday, 22 May 2023 14:15 (15 minutes)

Transport of species in porous media plays a crucial role in a variety of fields, including environmental engineering, geochemistry, and biology. Understanding the movement of species such as contaminants, nutrients, and microorganisms through porous media is essential for predicting and mitigating the impacts of human activities on the environment, as well as for developing effective remediation strategies [1]. For example, in the field of environmental engineering, knowledge of species transport in porous materials is essential for designing effective remediation strategies for contaminated soil and groundwater. In other applications such as water treatment, understanding the transport of nutrients and contaminants in porous media can help in the design of filtration systems and the optimization of treatment processes [2]. Additionally, research on transport of CO_2 in porous media is crucial for developing and implementing effective strategies for carbon sequestration in aquifers, which is a key component of efforts to mitigate climate change [3]. In general terms, the study of transport of species in porous media has the potential to significantly improve the effectiveness and efficiency of a wide range of environmental and engineering technologies.

In this study, we investigate the behavior of $A + B \rightarrow C$ reaction-diffusion chemical fronts in a finite radial geometry where the chemical species A and B are initially separated in space. In addition to the time properties found for rectilinear ([4]-[6]), and radial ([7]) geometries, we describe the dynamics of the spatial position of the reaction front (AB) which strongly depends on the initial parameters such as the ratio of initial concentrations ($\gamma = B_0/A_0$), ratio of diffusion coefficients ($\delta = D_B/D_A$), and the size of the geometry (R). We performed simulations and numerical analysis to predict the dynamics of the front and compared our results to experimental observations performed in gel and liquid systems.

Unlike previous studies done in infinitely extended domains, our results show that the reaction front could remain stationary at any spatial position depending only on the initial conditions. With the aforementioned numerical analysis, we are able to predict the short, medium, and long-time dynamics of the reaction front.

Our findings provide new insights into the behavior of $A + B \rightarrow C$ chemical fronts in finite radial geometry. By better understanding these dynamics, we can improve our ability to control and manipulate chemical reactions in more complex settings.

Participation

In-Person

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Session Classification: MS21

Track Classification: (MS21) Non-linear effects in flow and transport through porous media