Joint Condensed Matter and Center for Soft Matter and Biological Physics Seminar

In Person and Virtual

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"Chemical Fronts and the Effects of Convection"

Monday, March 28, 2022

4:00pm – 5:00pm

In Person: 304 Robeson Hall

Zoom Link: https://virginiatech.zoom.us/j/84041386169

Chemical fronts are spatially localized reaction zones driven by reaction and diffusion processes. In this talk, two classes of chemical fronts will be presented: ***bimolecular*** and (***thermal) polymerization*** fronts. A bimolecular front appears when two species A and B are initially separated in space, diffuse and react upon contact according to an elementary reactive event, $A + B \rightarrow C$. Such $A + B \rightarrow C$ fronts are therefore sustained by reaction and *mass diffusion.* On the other hand, thermal polymerization fronts are driven by *heat diffusion* and the exothermic polymerization whose reaction rate increases with temperature following Arrhenius' dependence.

In experiments, spontaneous hydrodynamic flows (convection) are typically observed to affect the chemical dynamics. In particular, $A + B \rightarrow C$ fronts have been experimentally observed to move faster than in experiments performed in gels or in microfluidic reactors; hence, breaking predictions from (mean-field) reaction-diffusion models. In the first part of the talk, we will analyze theoretically and numerically the effects of Marangoni stresses on bimolecular fronts. Such stresses are to be expected when systems are open to the air due to variation of surface tension along the air/liquid interface. In the second part of the talk, we will focus on the effects of buoyancy convection on polymerization fronts. The system is assumed to be closed so that to prevent any Marangoni effect. Buoyancy currents are then expected to be observed due to changes in density between the hot polymer and the cold reactants mixture in the gravity field.

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