Phase Field Modeling of Phase Separation and Dendrite Growth

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Abstract

A large variety of applications in environmental, petroleum and chemical engineering involve multiphase flow. Examples include fluid flow in presence of bubbles/droplets, phase separation of immiscible fluids and wetting phenomena. Multiphase flow is characterised by the presence of an interface which separates the two fluids. Such an interface can either be modelled as a sharp two-dimensional surface, whose location needs to be tracked during the motion, or as a three-dimensional volume of finite thickness, wherein fluid properties change continuously from their value in the bulk of one phase to the bulk of the second phase. The latter approach is called phase field modelling and allows for the modelling of interfacial phenomena starting from free energy functionals, without a-priori assumptions about the shape of the interface.

This study shows the implementation of a phase field model by using the General Form PDE interface of COMSOL Multiphysics®. The model solves for both energy and species conservation according to the Cahn-Hilliard equation. Notably, the free energy functional in the phase field approach generates a fourth-order PDE for the species molar fraction. We show that this can be easily handled in COMSOL Multiphysics® by adding an auxiliary variable, defined as the Laplacian of the molar fraction, thus resulting in two coupled second-order PDEs for species conservation. We discuss the requirements for obtaining mesh-independent results, showing that a structured mesh with spacing at least half the characteristic thickness of the interface is sufficient. Compared to an in-house Fortran code, which uses forward Euler time stepping, the implicit time-dependent solver of COMSOL Multiphysics® allows for a significant reduction in the computational time by over an order of magnitude, enabling simulation with logarithmically-spaced time steps. On the other hand, the memory requirements of COMSOL Multiphysics® are larger.

The model is used to analyse the spinodal decomposition of a viscous binary mixture with composition-dependent heat conductivities by applying either different temperatures at the lateral walls or by imposing a heat flux at the wall. For a binary mixture with equal molar fraction of the species, simulations show that phase separation starts from the cooler wall and evolves by generating bi-continuous dendrites of the two phases. The effect of the ratio of species conductivity as well as of conductivity/diffusivity ratio on dendrite orientation is investigated, showing that dendrites do not necessarily align along the temperature gradient. With precautionary analogy and extrapolations, these results shed light on the different topology of dendrite formation in lithium batteries for different current densities.

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Figures used in the abstract

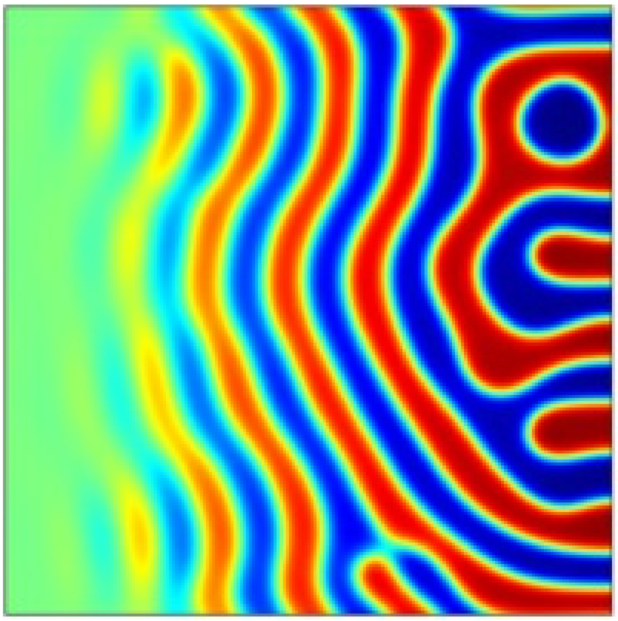

Figure 1: Phase separation of a binary mixture with composition-dependent conductivities under a horizontal thermal gradient.