Phase Field Modeling of Phase Separation and Dendrite Growth

A. Bertei[1], A. Lamorgese[2], R. Mauri[1], B. Tellini[2]
1. Department of Civil and Industrial Engineering, University of Pisa, Pisa, Italy
2. Department of Energy, Systems, Territory and Construction Engineering, University of Pisa, Pisa, Italy

INTRODUCTION: Phase separation occurs when a mixture of two miscible species, A and B, is cooled below its critical temperature. In such situation, two phases emerge from the mixture: a phase rich in component A and a phase rich in component B. The boundary between the two phases can be modelled either as a sharp interface or as a diffuse interface, wherein intrinsic properties vary smoothly. The latter approach is called phase field modelling and enables simulation of phase separation without a-priori assumptions about the interface.

Here we show the implementation of a phase field model of a binary mixture under a temperature gradient for different species thermal conductivities and conductivity/diffusivity ratios [1].

COMPUTATIONAL METHODS: The model is implemented by using the General Form PDE interface in COMSOL Multiphysics®. We consider a binary regular mixture of species having same molecular weight, density, heat capacity and diffusivity but different thermal conductivities $\kappa_B/\kappa_A = \lambda = 0.01$.

The model consists of two conservation equations: the conservation of species A (Eq. (1)), whose molar fraction is denoted with ϕ, and the conservation of energy (Eq. (2)):

$$\rho \frac{\partial \phi}{\partial t} + \nabla \cdot J_\phi = 0 \quad \text{(1a)} \qquad J_\phi = -\rho D \phi (1-\phi) \left[\nabla \tilde{\mu}_{AB} \right]_T \quad \text{(1b)}$$

$$\tilde{\mu}_{AB} = \ln \frac{\phi}{1-\phi} + \Psi(1-2\phi) - \hat{a}^2 \Psi \nabla^2 \phi \quad \text{(1c)}$$

$$\rho c \frac{\partial T}{\partial t} + \nabla \cdot J_q = 0 \quad \text{(2a)} \qquad J_q = -\kappa \left(\phi + \lambda (1-\phi) \right) \nabla T \quad \text{(2b)}$$

Notably, Eq. (1) represents a fourth-order PDE in the variable ϕ. In order to implement it, an additional balance equation in the variable u is introduced:

$$u \overset{\Delta}{=} \nabla^2 \phi \Rightarrow \nabla \cdot J_u = u \quad \text{(3a)} \qquad J_u = \nabla u \quad \text{(3b)}$$

The model is implemented in a square domain in dimensionless form upon the following change of variables and definitions:

$$\tilde{x} = \frac{x}{\hat{a}} \quad \text{(4a)} \qquad \tilde{t} = \frac{Dt}{\hat{a}^2} \quad \text{(4b)} \qquad \Psi = \frac{2T_C}{T} \quad \text{(4c)} \qquad Le = \frac{\kappa}{\rho c D} \quad \text{(4d)}$$

Periodic conditions at the top and bottom boundaries are set. Different temperatures, as Ψ_l and Ψ_r, are imposed at lateral boundaries, no flux is imposed for species transport. A uniform $\Psi_0 < 2$ is set as initial condition while a random noise initializes ϕ around ϕ_0.

RESULTS: Simulations show that phase separation always starts from the cooler boundary, which is the right one. When heat transport is slower than species transport (i.e., $Le < 1$), dendrites grow horizontally along the temperature gradient (Fig. 1). At the steady-state such a configuration allows for the maximum heat flux to be transferred between the walls.

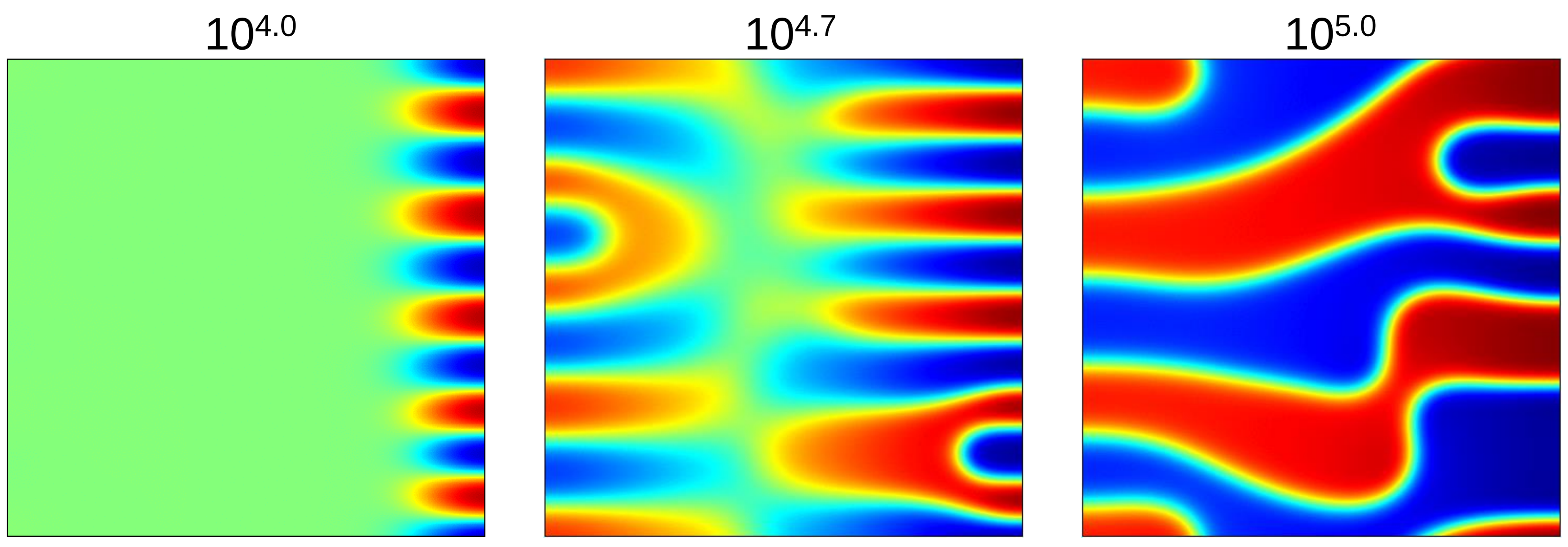

Figure 1. Dynamics of phase separation for $Le = 0.1$ and $\phi_0 = 0.5$ at different dimensionless times.

On the other hand, for $Le > 1$, the dynamics is different: while the steady-state is still characterized by horizontal dendrites, phase separation initially starts along vertical stripes, perpendicularly to the temperature gradient (Fig. 2). Such a pattern holds also for $\phi_0 \neq 0.5$, with bubble nucleation along vertical stripes (Fig. 3).

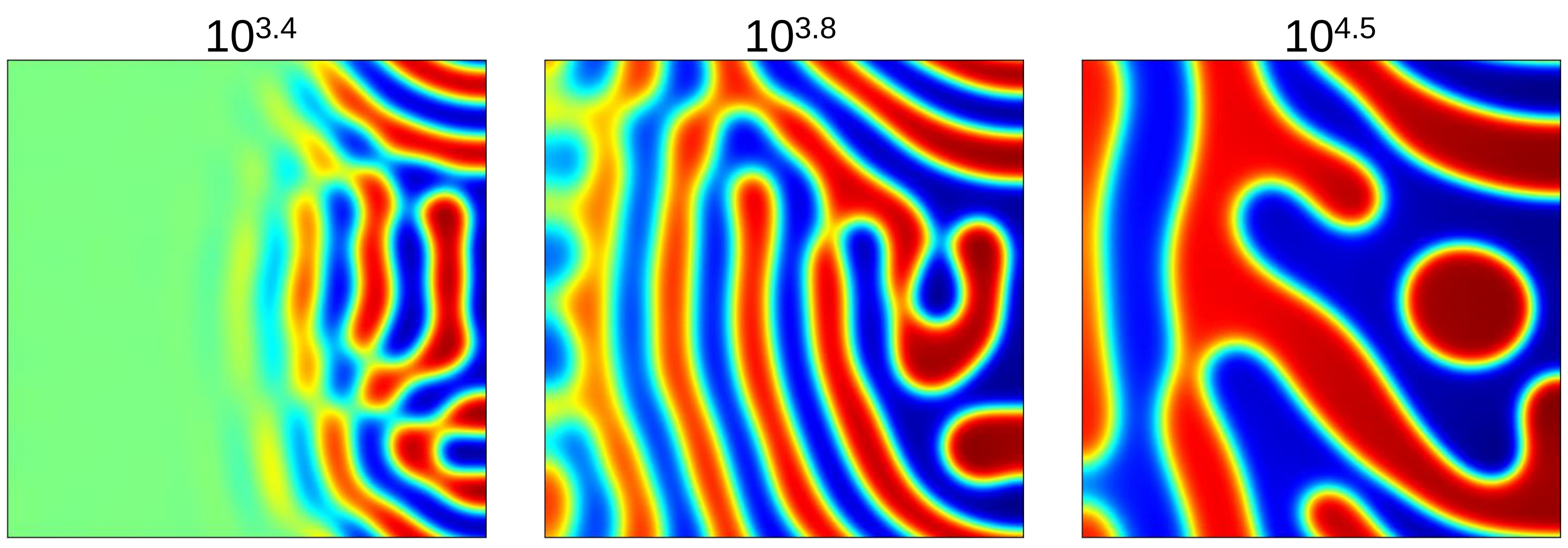

Figure 2. Dynamics of phase separation for $Le = 10$ and $\phi_0 = 0.5$.

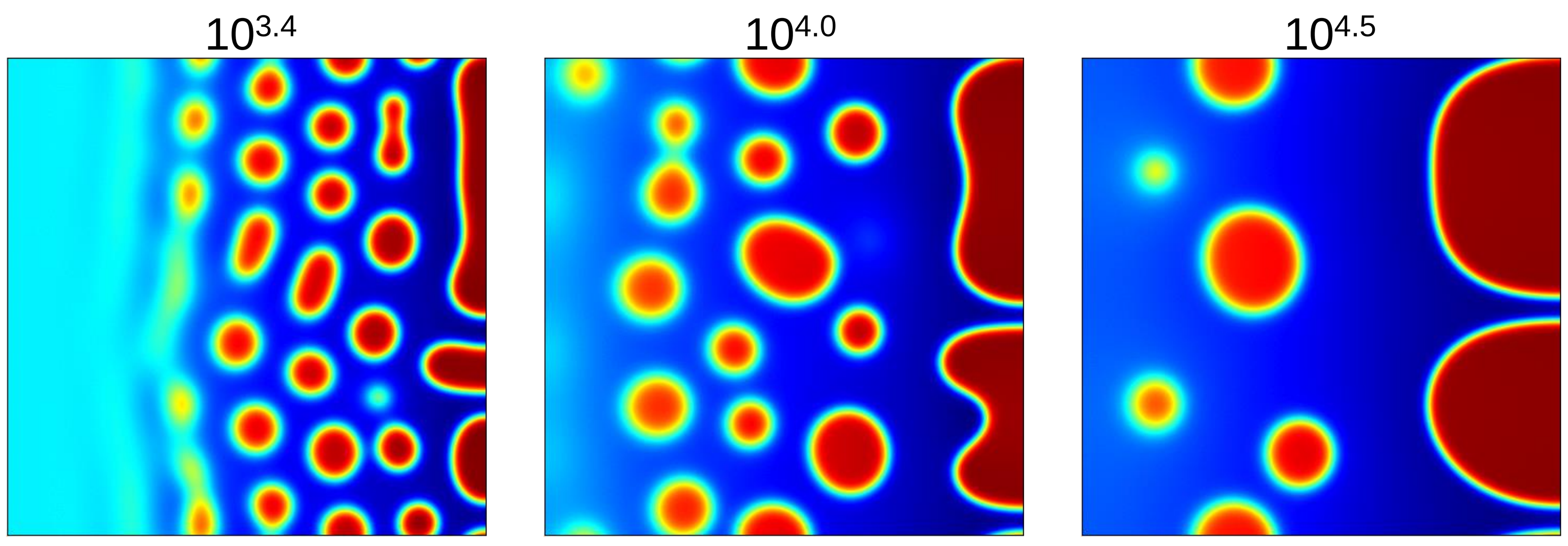

Figure 3. Dynamics of phase separation for $Le = 10$ and $\phi_0 = 0.4$.

CONCLUSIONS: The steady-state of phase separation of species with different thermal conductivities corresponds to horizontal stripes, which enable maximization of heat flux. However, when heat transport is faster than mass transport, dendrites initially align perpendicular to the temperature gradient.

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