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► **To cite this version:**

Domenico Borzacchiello, Adrien Leygue, Francisco Chinesta. A spectral volume-penalisation method for thermal fluid-structure interaction in phase-separating binary systems. 2nd ECCOMAS Young Investigators Conference (YIC 2013), Sep 2013, Bordeaux, France. hal-00855863

HAL Id: hal-00855863

<https://hal.science/hal-00855863>

Submitted on 30 Aug 2013

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A spectral volume-penalisation method for thermal fluid-structure interaction in phase-separating binary systems

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Abstract. *Spinodal decomposition of highly viscous binary mixtures near the critical composition is well described by the Cahn-Hilliard equation. In this short communication we present a model that introduces the thermal effects due to the presence of a solid structure immersed in a phase-separating mixture. The presence of solid boundaries is taken into account by means of a volume-penalisation method based on the phase-field formalism. Numerical experiments are carried out to show the influence of the temperature on the final morphology of the system.*

Keywords: thermal phase separation; volume-penalisation; cahn-hilliard equation.

1 INTRODUCTION

Phase demixing of binary solutions with critical or nearly-critical compositions can be accurately described by the Cahn-Hilliard equation (CH). According to this model, the phase separation is driven by the gradients of a generalized chemical potential that can be formally derived from a double well free energy function, [1].

Dimensional analysis [2] and numerical experiments [3] have shown that phase-separating systems described by the CH equation exhibit a dynamical scaling behaviour, that is the morphology of the system at a given time is statistically equivalent to the morphology at a previous time under an appropriate change of spatial scale. The characteristic length describing such scale is known to grow as the power 1/3 of time, meaning that the separation process never reaches an equilibrium in unbounded domains or alternatively that equilibrium is only reached when the characteristic length scale becomes of the same order of magnitude as the macroscopic size of the system. At this stage the separation is influenced by the presence of the boundaries.

The introduction of a temperature dependence in both the mobility and the miscibility of upper critical solution temperature (UCST) systems allows equilibrium at smaller scales since the latter results from the competition between the phase separation process and the rate at which the solution is quenched.

The determination of the morphology in UCST systems is a problem of major interest in the field of material processing technologies since the mechanical properties of composite materials are greatly influenced by the phase distribution at microscopic scale. Furthermore, thermal interactions between a phase separating solution and an immersed solid structure may produce temperature gradients and consequently compositional and structural gradients. As a result all the properties that are sensitive to these characteristics also display gradients across the system. This feature is particularly attractive since it might allow to locally tune up a specific property by controlling the temperature field.

In this short paper we discuss a model including temperature effects in phase separation and we present a numerical procedure to solve the CH equation for the case of weak thermal coupling with solid boundaries. The method proposed in section 2 relies on the Fourier Spectral Method (FSM) and thus retains the computational advantages typical of spectral methods while relying on a volume penalisation technique to take into account for the presence of solid boundaries inside the domain. In section 3, the case of longitudinal fibres immersed in a two-phase medium

is analysed, while conclusions are drawn in section 4.

2 MODEL FOR THERMALLY INDUCED PHASE SEPARATION

The volume penalisation method that we present in this section is based on the assumption that the presence of solid boundaries in a binary separating solution can be circumvented by considering the whole system as a ternary system characterized by the presence of an artificially diffused interface between the solid and liquid phases in the limit of small thickness of said interface. In this way the problem can be reformulated through a phase-field approach eliminating the complexity introduced by the domain topology in presence of solid boundaries.

2.1 Governing equations

As in the CH equation for binary solutions the phase-field formalism consists in defining a free energy density function, which for ternary system reads as:

$$f(c_1, c_2, c_3) = c_1 c_2 + c_2 c_3 + c_3 c_1 \quad (1)$$

where c_i is the volume fraction of the i -th species. The temporal evolution of each phase is governed by the equations:

$$\frac{\partial c_i}{\partial t} = \nabla D_i \cdot \nabla \left(\frac{\partial f}{\partial c_i} + \epsilon^2 \Delta c_i \right) + \xi \quad (2)$$

where $i = 1, 2, 3$, D_i is the mobility, ϵ is an interaction length determining the interface width and ξ is a Lagrange multiplier used to ensure that $c_1 + c_2 + c_3 = 1$ everywhere in the solution. Assuming 3 as the solid phase, $D_3 = 0$ and $D_1 = D_2 = m_0 (1 - c_3)$. The latter condition is the volume penalisation equivalent of the Neumann condition for the chemical potential $\partial_n \mu_i = 0$ prescribing no phase diffusion through solid walls. Replacing $c_2 = 1 - c_1 - c_3$ in the equation for c_1 and $c_1 = 1 - c_2 - c_3$ in the equation for c_2 , we obtain two constrained equations (having the same formal expression) to be solved simultaneously.

The miscibility dependence on temperature is introduced through a parameter $\chi = T_{cr}/T$, with T_{cr} the critical temperature, while the mobility is modelled as $D = D_1 = D_2 = \max[m_0 (1 - c_3) (T - T_s), 0]$ where T_s can be seen as the temperature at which the solution changes into a solid-like state.

The non-dimensionalisation of eq. (2) leads to the following expression:

$$\frac{\partial \phi_i}{\partial t} = \nabla D \cdot \nabla [\phi_i^3 + g_2(\phi_3) \phi_i^2 + g_1(\phi_3) \phi_i + g_0(\phi_3) - \Delta \phi_i] + \xi \quad (3)$$

With $i = 1, 2$, $g_0 = \frac{1}{2}(\phi_3 + 1)(\phi_3^2 + 3\phi_3)$, $g_2 = \frac{3}{2}(\phi_3 + 1)$ and $g_1 = \frac{9}{16}\chi\phi_3^2 + (3\chi/4 + 2)\phi_3 - \frac{21}{16}\chi + 5$. Note that the non-dimensional variable ϕ denotes the normalised deviation from the critical point concentration and is defined over the interval $[-1, 1]$. For $\phi_3 = -1$, that is in the fluid phase, equation (3) assumes the same form as the traditional CH equation.

The equation for the temperature reads as follows:

$$\frac{\partial T}{\partial t} = Le \nabla \cdot \kappa \nabla T + \frac{1}{C} (1 - \phi_3) (1 - \phi_1^2) \frac{\partial \phi_1}{\partial t} - \lambda T \quad (4)$$

Where $Le = \alpha/m_0$, is the Lewis number expressing the ratio between the thermal diffusivity and the mass diffusivity, while κ is the non-dimensional thermal conductivity. The second term in the right hand side of equation (4) expresses the energy dissipation due to the enthalpy of mixing and depends on the inverse of the non-dimensional specific heat C . Finally, the last term is an artificial source term introduced to control the cooling rate.

2.2 Numerical method

The model presented in the previous section is completed by the further assumptions that the two phase-separating components, 1 and 2, have the same thermal properties and that the heat produced by the phase separation reaction is negligible. These two hypothesis are fairly reasonable for polymeric materials for which the differences in the thermal conductivities are small and $Le \gg C^{-1}$ by several orders of magnitude. As a direct consequence, the thermal conductivity is only function of ϕ_3 and the equation for the temperature can be solved separately from the equations for $\phi_{1,2}$.

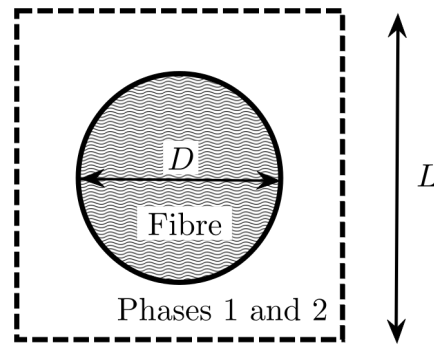


Figure 1: Schematic of the periodic two-dimensional system consisting of the fibre section immersed in a bicomponent phase-separating system.

For both equations (3) and (4), a first order implicit-explicit splitting time stepping scheme is adopted to enhance numerical stability. The latter is inspired by the scheme proposed in [4] for the CH equation.

Since the implicit part corresponds to a linear elliptic operator with constant coefficients, the linear system arising from the spectral method discretisation can be efficiently solved by means of the Fast Fourier Transform and its inverse. The solution for the phase field is composed of two parts. In a first prediction step, equation (3) is solved for $\phi_{1,2}^*$ assuming $\xi = 0$, while in the correction step the Lagrange multiplier is determined as $\xi = -(1 + \phi_3 + \phi_1^* + \phi_2^*)/2$ and $\phi_1 = \phi_1^* + \xi$, $\phi_2 = \phi_2^* + \xi$.

3 SPINODAL DECOMPOSITION OF A BINARY SOLUTION WITH IMMERSed FIBRES

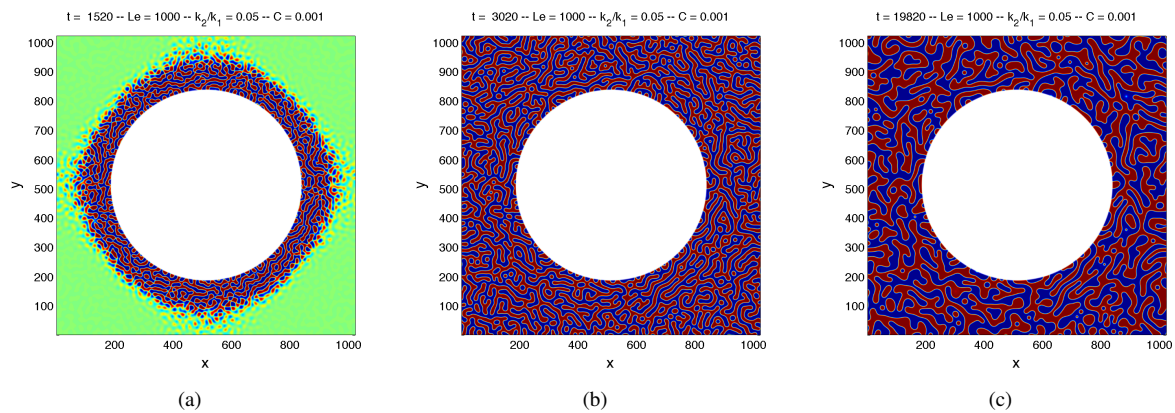


Figure 2: Phase separation evolution for $Le = 1000$ at $t = 1520$ (a), $t = 3020$ (b), $t = 19820$ (c).

In this section we consider, as a numerical application, the determination of the final morphology resulting from the phase separation process of a binary solution in presence of longitudinal fibres. The numerical simulations are carried out in two dimensions, in the plane orthogonal to the fibres as sketched in fig. 1, while the presence of multiple fibres is taken into account by imposing periodic boundary conditions. This simplified model can be descriptive of the thermal effects in a bicomponent polymeric matrix with immersed carbon micro-fibres. Since the conductivity of carbon fibres is in general at least one order of magnitude greater than that of polymeric resins, the conductivity ratio is taken as $1/20$. The control parameter λ in equation (4) is taken as $10^{-3}\kappa$. This is done in order to model the fact that the fibres cool down more rapidly than the surrounding medium. With reference to fig. 1, the Cahn number of the system is defined as $Cn = (L - D)/\epsilon$ and expresses the ratio between the inter-fibre distance and the thickness of the interface between the phases 1 and 2. The latter represents the phase separation natural length scale. In our simulations $Cn = 374$, $L = 1024$, $D = 650$ and $\Delta x = \Delta y = 1$. As initial condition we assume a homogeneous solution with critical composition (i.e. $\phi_1 = \phi_2 = 0$) at $T = T_{cr}$.

To investigate the influence of thermal effects in phase separation we carried out simulations for different values of

the Lewis number. For $Le = 1000$, that is when the thermal diffusion is faster than the phase separation, the solution is rapidly cooled and the separation process occurs almost uniformly around the fibre. The observed static contact angle between the two phases at the solid wall is of 90. This is a direct consequence of the choice for the free energy density expressed by the function (1), in which the surface tensions between the three phases are implicitly taken as equal.

For $Le = 1$ the thermal and phase separation characteristic times are of the same order of magnitude. The phase demixing process results in the formation of domains that are parallel to the isothermal lines, as observed in fig. 3. This result is also confirmed by the numerical simulations in [5]. The formation of this particular morphology is a consequence of the fact that the isothermal line corresponding to $T = T_{cr}$, delimiting the unstable region around the fibre where the decomposition takes place, propagates at the same velocity at which the two phases separate. This means that as the unstable region radially expands, the phase separation instantaneously attains equilibrium, generating a morphology pattern that aligns with the isothermal lines.

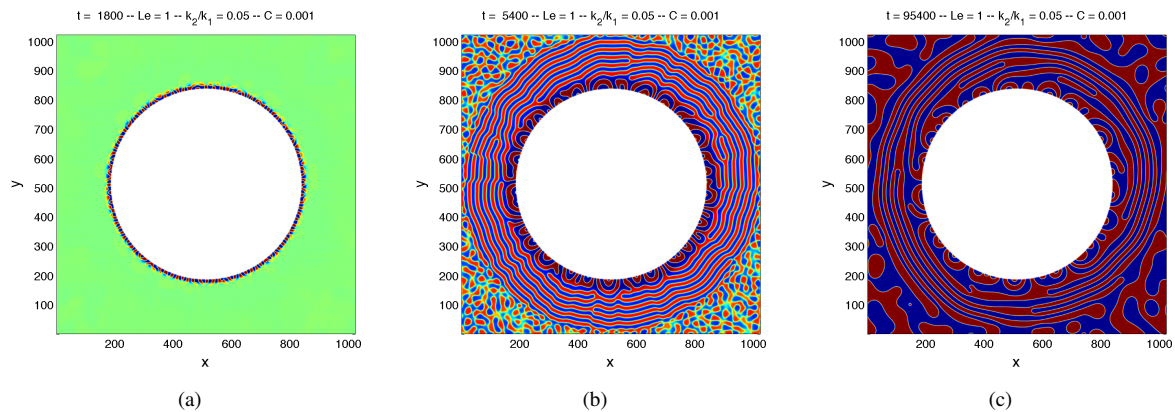


Figure 3: Phase separation evolution for $Le = 1$ at $t = 1800$ (a), $t = 5400$ (b), $t = 95400$ (c).

4 CONCLUSIONS

We presented a volume-penalisation spectral method that can be used to solve the Cahn-Hilliard equation in presence of immersed obstacles with natural boundary conditions on the solid boundaries, i.e. homogeneous Neumann conditions for the phase and the chemical potential. More general wall affinity conditions can be assigned by specifically selecting the form of the free energy density function. We used the proposed model to describe the effects of temperature in phase separation of fibre-reinforced binary mixtures and we showed the role of the Lewis number in determining the final morphology pattern. The dependence of the morphology on fibre diameter and spacing is the subject of an ongoing investigation.

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