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SHARP INTERFACE LIMIT OF A HOMOGENIZED PHASE FIELD MODEL FOR PHASE TRANSITIONS IN POROUS MEDIA

MARTIN HÖPKER

Abstract. A homogenized phase field model for phase transitions in porous media is considered. By making use of the method of formal asymptotic expansion with respect to the interface thickness, a sharp interface limit problem is derived. This limit problem turns out to be similar to the classical Stefan problem with surface tension and kinetic undercooling.

1. Introduction

The study of the phase change between water and ice in porous media plays a vital role in the understanding of important phenomena like the frost attack on concrete or the thawing of permafrost soil. In [8], a mathematical microscale model of this process, based on the standard Caginalp phase field model for phase transitions, is presented and homogenized via two-scale convergence. Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain that represents a porous body, and let $S := (0, T)$ be a time interval. The homogenized problem is of the form: Find u, θ, and χ such that

$$|Z^{\rm s}|\rho_{\rm s} u' - \operatorname{div}(P^{\rm s}\nabla u) + |\Gamma|\kappa_{RI}(u - \theta) = 0, \tag{1.1a}$$

$$|Z^{\rm p}|\rho_{\rm p}\theta' + |Z^{\rm p}|\frac{\lambda}{2}\chi' - \operatorname{div}(P^{\rm p}\nabla\theta) + |\Gamma|\kappa_{RI}(\theta - u) = 0, \tag{1.1b}$$

$$|Z^{\rm p}|\alpha\xi^2\chi' - \xi^2\operatorname{div}(P\nabla\chi) + |Z^{\rm p}|\frac{1}{2a}(\chi^3 - \chi) = |Z^{\rm p}|2\theta \tag{1.1c}$$

in $S \times \Omega$, supplemented by exchange boundary conditions and initial conditions.

In the system (1.1), u and θ are the effective temperatures in the solid matrix and in the pore space of the porous medium, respectively, and χ is the effective phase field variable. The constant parameter ξ represents the small interface thickness of the phase field. The coefficients $\rho_{\rm s}, \rho_{\rm p}, \kappa_{RI}, \lambda, \alpha, a$ are positive and constant parameters, and $P^{\rm s}$, $P^{\rm p}$, P are homogenized, positive definite tensors. The constants $|Z^{\rm s}|$ and $|Z^{\rm p}|$ represent the volume of the solid matrix and of the pore space in the reference cell in the homogenization, and $|\Gamma|$ denotes the surface measure of their interface. For the details of the modeling and the homogenization that lead to (1.1), we refer to [8]. We also refer to [4], [1], and [12] for an introduction to

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phase field models for phase transitions, as well as to [10] for the similar concept of *mushy regions*.

In this article, we apply the method of formal asymptotic expansion, with respect to the interface thickness ξ, to derive a sharp interface model from the homogenized phase field model (1.1). To this end, we follow the lines of [1], where the main difference lies in the homogenized tensor P in equation (1.1c), which replaces the identity matrix from the standard phase field model. The sharp interface model turns out to be similar to the classical *Stefan problem* (see, e.g., [11], [9], [12], and [5]) with surface tension and kinetic undercooling but involves some additional terms.

This article is organized as follows: In 2, the system (1.1) is appropriately scaled. In 3, we introduce a local coordinate system near the phase interface. Sections 4, 5 are concerned with the asymptotic expansions of the variables u, θ, and χ outside of and near the interface. Limit equations are derived from the system (1.1) by neglecting terms of high order. Finally, in 6, the full sharp interface limit model is stated.

2. Scaling

Similarly as in [1, Section IV], we will consider the limit $\xi \to 0$ and $a \to 0$ with fixed $\frac{\xi}{\sqrt{a}}$. To this end, we introduce the scaling $\epsilon = \xi^2$ and $\frac{\epsilon}{a} = C_0$ in equation (1.1c), which yields

$$|Z^{\mathrm{p}}|\alpha\epsilon^2\chi' - \epsilon^2 \operatorname{div}(P\nabla\chi) + |Z^{\mathrm{p}}|\frac{C_0}{2}(\chi^3 - \chi) = \epsilon|Z^{\mathrm{p}}|2\theta. \tag{2.1}$$

We define $g(\chi) := |Z^{\mathrm{p}}|\frac{C_0}{2}(\chi - \chi^3)$ and, for simplicity, also rename the constants in the equations (1.1a), (1.1b), and (2.1) such that we obtain the scaled system

$$\rho_{\mathrm{s}} u' - \operatorname{div}(P^{\mathrm{s}}\nabla u) + \kappa_{RI}(u - \theta) = 0 \tag{2.2a}$$

$$\rho_{\mathrm{p}}\theta' + \frac{\lambda}{2}\chi' - \operatorname{div}(P^{\mathrm{p}}\nabla\theta) + \kappa_{RI}(\theta - u) = 0. \tag{2.2b}$$

$$\alpha\epsilon^2\chi' - \epsilon^2 \operatorname{div}(P\nabla\chi) = g(\chi) + \epsilon\beta\theta \quad \text{in } \Omega \times S. \tag{2.2c}$$

Note that θ, χ, and u depend on the scaling parameter ϵ.

Remark 2.1. Different scalings of phase field models may yield different asymptotic limits. See, e.g., [1] and [2], where various limit models are derived from the Caginalp phase field model.

3. Interface and Local Coordinates

Using the phase field variable χ, we define the interface between the solid and the liquid phase at time t to be given by the set

$$\Gamma(t,\epsilon) := \{x \in \Omega : \chi(t,x) = 0\}.$$

In the following, we assume that $\Gamma(t,\epsilon)$ is a closed, connected, and sufficiently smooth surface. A point $x \in \Omega$ near $\Gamma(t,\epsilon)$ can then be represented in the local orthogonal coordinate system (r, s_1, s_2), which is often used when deriving sharp limits of phase field models (see, e.g., [1, 3, 7]): By $r(t,x,\epsilon)$, we denote the signed distance of x to the interface $\Gamma(t,\epsilon)$ (which is chosen positive if x lies in the liquid phase), and $s_1(t,x,\epsilon)$ and $s_2(t,x,\epsilon)$ are measures of arc length along $\Gamma(t,\epsilon)$ from a reference point. We write $s = (s_1\ s_2)$. The coordinate system (r,s) satisfies

$|\nabla r| = 1$ and $\Delta r = \kappa$ near $\Gamma(t,\epsilon)$, where κ is the mean curvature of $\Gamma(t,\epsilon)$ (The sign of the mean curvature is chosen such that $\kappa > 0$ for a strictly convex solid phase.). Furthermore, $\nabla r \cdot \nabla s_i = 0$ for $i = 1, 2$. We assume the following asymptotic expansions of the coordinates:

$$\begin{aligned} r(t,x,\epsilon) &= r^0(t,x) + \epsilon r^1(t,x) + \epsilon^2 r^2(t,x) + \dots, \\ s_i(t,x,\epsilon) &= s_i^0(t,x) + \epsilon s_i^1(t,x) + \epsilon^2 s_i^2(t,x) + \dots, \quad \text{for } i = 1, 2. \end{aligned}$$

We assume that, for $\varepsilon \to 0$, the interfaces $\Gamma(t,\epsilon)$ converge (uniformly in distance) to a closed, connected, and smooth interface $\Gamma^0(t)$ that has a neighbourhood parametrized by r^0 and $s^0 = (s_1^0\ s_2^0)$. The liquid and the solid phase, which are seperated by $\Gamma^0(t)$, are denoted by $\Omega_l(t)$ and $\Omega_s(t)$, respectively. By $\vec{n}(t,x)$, we denote the unit normal vector on $\Gamma^0(t)$ at point x into the liquid phase $\Omega_l(t)$.

Let $A \in \mathbb{R}^{3\times 3}$ be a constant and symmetric matrix, and let $u\colon S \times \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}$. We consider the coordinate change

$$u(t,x,\epsilon) = \tilde{u}(t,r,s,\epsilon).$$

For later reference, we note that this transformation yields

$$\begin{aligned} \operatorname{div}(A\nabla u) = {} & \frac{\partial^2 \tilde{u}}{\partial r^2} \nabla r^{\mathrm{T}} A \nabla r + \frac{\partial \tilde{u}}{\partial r} \operatorname{div}(A\nabla r) + 2\sum_{l=1}^{2} \frac{\partial^2 \tilde{u}}{\partial r \partial s_l} \nabla s_l^{\mathrm{T}} A \nabla r \\ & + \sum_{l=1}^{2} \frac{\partial \tilde{u}}{\partial s_l} \operatorname{div}(A\nabla s_l) + \sum_{l,m=1}^{2} \frac{\partial^2 \tilde{u}}{\partial s_l \partial s_m} \nabla s_m^{\mathrm{T}} A \nabla s_l \end{aligned} \tag{3.1}$$

and

$$\frac{\partial u}{\partial t} = \frac{\partial \tilde{u}}{\partial t} + \frac{\partial r}{\partial t}\frac{\partial \tilde{u}}{\partial r} + \sum_{l=1}^{2} \frac{\partial s_l}{\partial t}\frac{\partial \tilde{u}}{\partial s_l}. \tag{3.2}$$

4. Outer Expansions

Outside of $\Gamma(t,\epsilon)$, we assume the following *outer expansions* in the cartesian coordinate system

$$u(t,x,\epsilon) = u^0(t,x) + \epsilon u^1(t,x) + \epsilon^2 u^2(t,x) + \dots, \tag{4.1a}$$

$$\theta(t,x,\epsilon) = \theta^0(t,x) + \epsilon \theta^1(t,x) + \epsilon^2 \theta^2(t,x) + \dots, \tag{4.1b}$$

$$\chi(t,x,\epsilon) = \chi^0(t,x) + \epsilon \chi^1(t,x) + \epsilon^2 \chi^2(t,x) + \dots. \tag{4.1c}$$

The terms on the right-hand side of the equations (4.1b) and (4.1c) are assumed to be twice differentiable in $\Omega\backslash\Gamma^0(t)$ but may be discontinuous across the limit phase interface $\Gamma^0(t)$. Since the variable u is not directly connected to the phase change, we assume the u_k, for all $k \in \mathbb{N}$, to be twice differentiable in the whole domain Ω. From the order $\mathcal{O}(1)$ of (2.2a), we deduce the equation

$$\rho_{\mathrm{s}} {u^0}' - \operatorname{div}(P^{\mathrm{s}} \nabla u^0) + \kappa_{RI}(u^0 - \theta^0) = 0, \tag{4.2}$$

which is valid in the whole domain Ω. By using the expansion of χ, it is easy to obtain that

$$\begin{aligned} g(\chi) &= |Z^{\mathrm{p}}|\frac{C_0}{2}(\chi^0 - (\chi^0)^3) + \epsilon |Z^{\mathrm{p}}|\frac{C_0}{2}(\chi^1 - 3(\chi^0)^2\chi^1) + \mathcal{O}(\epsilon^2) \\ &= g(\chi^0) + \epsilon g'(\chi^0)\chi^1 + \mathcal{O}(\epsilon^2). \end{aligned} \tag{4.3}$$

Equations (2.2b) and (2.2c) thus yield the order $\mathcal{O}(1)$ equations

$$\rho_{\mathrm{p}}\theta^{0\prime} + \frac{\lambda}{2}\chi^{0\prime} - \operatorname{div}(P^{\mathrm{p}}\nabla\theta^0) + \kappa_{RI}(\theta^0 - u^0) = 0 \tag{4.4}$$

and

$$g(\chi^0) = 0, \tag{4.5}$$

respectively. Note that equation (4.4) is only valid on each side of $\Gamma^0(t)$, due to the possible discontinuity of θ^0 and χ^0 across $\Gamma^0(t)$. Equation (4.5) implies that χ^0 takes one of the constant values $0, 1$, or -1 on each side of $\Gamma^0(t)$. Hence, $\chi^{0\prime} = 0$, and we can thus deduce

$$\rho_{\mathrm{p}}\theta^{0\prime} - \operatorname{div}(P^{\mathrm{p}}\nabla\theta^0) + \kappa_{RI}(\theta^0 - u^0) = 0 \tag{4.6}$$

from (4.4), outside of $\Gamma^0(t)$.

Furthermore, we consider the coordinate change

$$\begin{aligned} u(t,x,\epsilon) &= \tilde{u}(t,r,s,\epsilon),\\ \theta(t,x,\epsilon) &= \tilde{\theta}(t,r,s,\epsilon),\\ \chi(t,x,\epsilon) &= \tilde{\chi}(t,r,s,\epsilon) \end{aligned}$$

and assume the following expansions to hold:

$$\begin{aligned} \tilde{u}(t,r,s,\epsilon) &= \tilde{u}^0(t,r,s) + \epsilon\tilde{u}^1(t,r,s) + \epsilon^2\tilde{u}^2(t,r,s) + \dots,\\ \tilde{\theta}(t,r,s,\epsilon) &= \tilde{\theta}^0(t,r,s) + \epsilon\tilde{\theta}^1(t,r,s) + \epsilon^2\tilde{\theta}^2(t,r,s) + \dots,\\ \tilde{\chi}(t,r,s,\epsilon) &= \tilde{\chi}^0(t,r,s) + \epsilon\tilde{\chi}^1(t,r,s) + \epsilon^2\tilde{\chi}^2(t,r,s) + \dots. \end{aligned}$$

5. Inner Expansions

In a neighbourhood of $\Gamma(t,\epsilon)$, we introduce a coordinate change, using the stretched variable $z := \frac{r}{\epsilon}$:

$$\begin{aligned} \tilde{u}(t,r,s,\epsilon) &= U(t,z,s,\epsilon),\\ \tilde{\theta}(t,r,s,\epsilon) &= \vartheta(t,z,s,\epsilon),\\ \tilde{\chi}(t,r,s,\epsilon) &= X(t,z,s,\epsilon), \end{aligned}$$

and assume the *inner expansions*

$$\begin{aligned} U(t,z,s,\epsilon) &= U^0(t,z,s) + \epsilon U^1(t,z,s) + \epsilon^2 U^2(t,z,s) + \dots,\\ \vartheta(t,z,s,\epsilon) &= \vartheta^0(t,z,s) + \epsilon\vartheta^1(t,z,s) + \epsilon^2\vartheta^2(t,z,s) + \dots,\\ X(t,z,s,\epsilon) &= X^0(t,z,s) + \epsilon X^1(t,z,s) + \epsilon^2 X^2(t,z,s) + \dots. \end{aligned}$$

In the context of the above coordinate change, we note that $\frac{\partial}{\partial r} = \frac{1}{\epsilon}\frac{\partial}{\partial z}$. By using the identities (3.1) and (3.2), we can thus rewrite equation (2.2b) as

$$\begin{aligned} &\rho_{\mathrm{p}}\frac{\partial\vartheta}{\partial t} + \frac{1}{\epsilon}\rho_{\mathrm{p}}\frac{\partial r}{\partial t}\frac{\partial\vartheta}{\partial z} + \rho_{\mathrm{p}}\sum_{l=1}^{2}\frac{\partial s_l}{\partial t}\frac{\partial\vartheta}{\partial s_l} + \frac{\lambda}{2}\frac{\partial X}{\partial t} + \frac{1}{\epsilon}\frac{\lambda}{2}\frac{\partial r}{\partial t}\frac{\partial X}{\partial z} + \frac{\lambda}{2}\sum_{l=1}^{2}\frac{\partial s_l}{\partial t}\frac{\partial X}{\partial s_l}\\ &- \frac{1}{\epsilon^2}\frac{\partial^2\vartheta}{\partial z^2}\nabla r^{\mathrm{T}}P^{\mathrm{p}}\nabla r - \frac{1}{\epsilon}\frac{\partial\vartheta}{\partial z}\operatorname{div}(P^{\mathrm{p}}\nabla r) - \frac{1}{\epsilon}2\sum_{l=1}^{2}\frac{\partial^2\vartheta}{\partial z\partial s_l}\nabla s_l^{\mathrm{T}}P^{\mathrm{p}}\nabla r\\ &- \sum_{l=1}^{2}\frac{\partial\vartheta}{\partial s_l}\operatorname{div}(P^{\mathrm{p}}\nabla s_l) - \sum_{l,m=1}^{2}\frac{\partial^2\vartheta}{\partial s_l\partial s_m}\nabla s_m^{\mathrm{T}}P^{\mathrm{p}}\nabla s_l + \kappa_{RI}(\vartheta - U) = 0. \end{aligned}$$

Multiplying by ϵ^2 yields

$$\begin{aligned}
&\epsilon^2\rho_{\mathrm{p}}\frac{\partial\vartheta}{\partial t}+\epsilon\rho_{\mathrm{p}}\frac{\partial r}{\partial t}\frac{\partial\vartheta}{\partial z}+\epsilon^2\rho_{\mathrm{p}}\sum_{l=1}^{2}\frac{\partial s_l}{\partial t}\frac{\partial\vartheta}{\partial s_l}+\epsilon^2\frac{\lambda}{2}\frac{\partial X}{\partial t}+\epsilon\frac{\lambda}{2}\frac{\partial r}{\partial t}\frac{\partial X}{\partial z}\\
&+\epsilon^2\frac{\lambda}{2}\sum_{l=1}^{2}\frac{\partial s_l}{\partial t}\frac{\partial X}{\partial s_l}-\frac{\partial^2\vartheta}{\partial z^2}\nabla r^{\mathrm{T}}P^{\mathrm{p}}\nabla r-\epsilon\frac{\partial\vartheta}{\partial z}\operatorname{div}(P^{\mathrm{p}}\nabla r)\\
&-\epsilon 2\sum_{l=1}^{2}\frac{\partial^2\vartheta}{\partial z\partial s_l}\nabla s_l^{\mathrm{T}}P^{\mathrm{p}}\nabla r-\epsilon^2\sum_{l=1}^{2}\frac{\partial\vartheta}{\partial s_l}\operatorname{div}(P^{\mathrm{p}}\nabla s_l)\\
&-\epsilon^2\sum_{l,m=1}^{2}\frac{\partial^2\vartheta}{\partial s_l\partial s_m}\nabla s_m^{\mathrm{T}}P^{\mathrm{p}}\nabla s_l+\epsilon^2\kappa_{RI}(\vartheta-U)=0.
\end{aligned}\tag{5.1}$$

By using the inner expansions, we deduce from the phase field equation (2.2c) that

$$\begin{aligned}
&\epsilon^2\alpha\frac{\partial X}{\partial t}+\epsilon\alpha\frac{\partial r}{\partial t}\frac{\partial X}{\partial z}+\epsilon^2\alpha\sum_{l=1}^{2}\frac{\partial s_l}{\partial t}\frac{\partial X}{\partial s_l}\\
&-\frac{\partial^2 X}{\partial z^2}\nabla r^{\mathrm{T}}P\nabla r-\epsilon\frac{\partial X}{\partial z}\operatorname{div}(P\nabla r)-\epsilon 2\sum_{l=1}^{2}\frac{\partial^2 X}{\partial z\partial s_l}\nabla s_l^{\mathrm{T}}P\nabla r\\
&-\epsilon^2\sum_{l=1}^{2}\frac{\partial X}{\partial s_l}\operatorname{div}(P\nabla s_l)-\epsilon^2\sum_{l,m=1}^{2}\frac{\partial^2 X}{\partial s_l\partial s_m}\nabla s_m^{\mathrm{T}}P\nabla s_l\\
&=g(X)+\epsilon\beta\vartheta.
\end{aligned}\tag{5.2}$$

Similarly as with equation (4.3), we obtain

$$g(X)=g(X^0)+\epsilon g'(X^0)X^1+\mathcal{O}(\epsilon^2).\tag{5.3}$$

The order $\mathcal{O}(1)$ of equation (5.1) yields

$$-\frac{\partial^2\vartheta^0}{\partial z^2}\nabla {r^0}^{\mathrm{T}}P^{\mathrm{p}}\nabla r^0=0.$$

From $|\nabla r|=1$, it follows that $\nabla r^0\neq 0$. Since P^{p} is positive definite, we can hence deduce

$$-\frac{\partial^2\vartheta^0}{\partial z^2}=0.$$

This yields $\vartheta^0(t,z,s)=a(t,s)z+b(t,s)$ with $a(t,s),b(t,s)\in\mathbb{R}$. We apply the matching condition (see, e.g., [1])

$$\tilde{\theta}^0(t,\Gamma^0_{\pm})=\lim_{z\to\pm\infty}\vartheta^0(t,z,s),\tag{5.4}$$

which connects the inner and the outer expansions. Here, we denote by $\tilde{\theta}^0(t,\Gamma^0_{\pm})$ the value of $\tilde{\theta}^0$ when approaching $\Gamma^0(t)$ from the liquid and the solid phase, respectively. From the natural assumption that $\tilde{\theta}^0$ is bounded at the interface $\Gamma^0(t)$, we deduce $a=0$ from the equation (5.4). Thus,

$$\vartheta^0(t,z,s)=b(t,s),\tag{5.5}$$

independently of z. Analogously to (5.4), we apply the matching condition

$$\lim_{z\to\pm\infty}X^0(t,z,s)=\tilde{\chi}^0(t,\Gamma^0_{\pm})=\pm 1.\tag{5.6}$$

We note that $X(t,0,s,\epsilon)=0$ by the definition of $\Gamma(t,\epsilon)$. It, thus, directly follows that

$$X^0(t,0,s)=0.$$

We now consider the $\mathcal{O}(\epsilon)$ balance of equation (5.1):

$$\begin{aligned}&\rho_{\rm p}\frac{\partial r^0}{\partial t}\frac{\partial \vartheta^0}{\partial z}+\frac{\lambda}{2}\frac{\partial r^0}{\partial t}\frac{\partial X^0}{\partial z}-2\frac{\partial^2\vartheta^0}{\partial z^2}{\nabla r^1}^{\rm T}P^{\rm p}\nabla r^0-\frac{\partial^2\vartheta^1}{\partial z^2}{\nabla r^0}^{\rm T}P^{\rm p}\nabla r^0\\&-\frac{\partial\vartheta^0}{\partial z}\operatorname{div}(P^{\rm p}\nabla r^0)-2\sum_{l=1}^2\frac{\partial^2\vartheta^0}{\partial z\partial s_l}{\nabla s_l^0}^{\rm T}P^{\rm p}\nabla r^0=0.\end{aligned}$$

Since ϑ^0 is constant with respect to the variable z, we obtain

$$\frac{\lambda}{2}\frac{\partial r^0}{\partial t}\frac{\partial X^0}{\partial z}=\frac{\partial^2\vartheta^1}{\partial z^2}{\nabla r^0}^{\rm T}P^{\rm p}\nabla r^0.$$

Thus, integration with respect to z yields

$$\frac{\lambda}{2}\frac{\partial r^0}{\partial t}X^0+c=\frac{\partial\vartheta^1}{\partial z}{\nabla r^0}^{\rm T}P^{\rm p}\nabla r^0,$$

where c may depend on t and s but not on z. In the following, we will apply the matching condition (see, e.g., [1])

$$\frac{\partial\tilde\theta^0}{\partial r}(t,\Gamma^0_\pm)=\lim_{z\to\pm\infty}\frac{\partial\vartheta^1}{\partial z}(t,z,s).$$

We calculate

$$\begin{aligned}\frac{\partial\tilde\theta^0}{\partial r}(t,\Gamma^0_\pm){\nabla r^0}^{\rm T}P^{\rm p}\nabla r^0&=\lim_{z\to\pm\infty}\frac{\partial\vartheta^1}{\partial z}{\nabla r^0}^{\rm T}P^{\rm p}\nabla r^0=\frac{\lambda}{2}\frac{\partial r^0}{\partial t}\lim_{z\to\pm\infty}X^0+c\\&=\pm\frac{\lambda}{2}\frac{\partial r^0}{\partial t}+c.\end{aligned}$$

Thus,

$$ {\nabla r^0}^{\rm T}P^{\rm p}\nabla r^0\Big[\frac{\partial\tilde\theta^0}{\partial r}\Big]_{\Gamma^0_\pm}=-\lambda V\quad\text{on }\Gamma^0(t), \tag{5.7}$$

where $V=-\frac{\partial r^0}{\partial t}$ is the normal velocity of $\Gamma^0(t)$ (in the direction $\vec n$) and $[\frac{\partial\tilde\theta^0}{\partial r}]_{\Gamma^0_\pm}=[\frac{\partial\theta^0}{\partial\vec n}]_{\Gamma^0_\pm}$ denotes the jump of the normal derivative $\frac{\partial\theta^0}{\partial\vec n}$ across $\Gamma^0(t)$.

We now consider the problem of order $\mathcal{O}(\epsilon)$ of equation (5.2):

$$\begin{aligned}&\alpha\frac{\partial r^0}{\partial t}\frac{\partial X^0}{\partial z}-2\frac{\partial^2X^0}{\partial z^2}{\nabla r^1}^{\rm T}P\nabla r^0-\frac{\partial^2X^1}{\partial z^2}{\nabla r^0}^{\rm T}P\nabla r^0\\&-\frac{\partial X^0}{\partial z}\operatorname{div}(P\nabla r^0)-2\sum_{l=1}^2\frac{\partial^2X^0}{\partial z\partial s_l}{\nabla s_l}^{0\,\rm T}P\nabla r^0\\&=g'(X^0)X^1+\beta\vartheta^0,\end{aligned}\tag{5.8}$$

to which we (see, e.g., [6]) add the boundary condition

$$\lim_{z\to\pm\infty}X^1(t,z,s)=0, \tag{5.9}$$

meaning that the phase field variable equals zero up to order ε. The order $\mathcal{O}(1)$ problem of equation (5.2) reads

$$\frac{\partial^2X^0}{\partial z^2}{\nabla r^0}^{\rm T}P\nabla r^0+g(X^0)=0,$$

from which we deduce, by differentiating,

$$\frac{\partial}{\partial z}\frac{\partial^2 X^0}{\partial z^2}\nabla {r^0}^{\mathrm{T}} P \nabla r^0 + g'(X^0)\frac{\partial X^0}{\partial z} = 0.$$

Thus, using integration by parts and the condition (5.9) (compare to the approach in [5, Section 7.9]), we obtain

$$\begin{aligned}
&\int_{\mathbb{R}} \Big(\frac{\partial^2 X^1}{\partial z^2}\nabla {r^0}^{\mathrm{T}} P\nabla r^0 + g'(X^0)X^1\Big)\frac{\partial X^0}{\partial z}\,\mathrm{d}z \\
&= \int_{\mathbb{R}} \frac{\partial^2 X^1}{\partial z^2}\nabla {r^0}^{\mathrm{T}} P\nabla r^0 \frac{\partial X^0}{\partial z} + g'(X^0)X^1\frac{\partial X^0}{\partial z}\,\mathrm{d}z \\
&= \int_{\mathbb{R}} X^1 \nabla {r^0}^{\mathrm{T}} P\nabla r^0 \frac{\partial}{\partial z}\frac{\partial^2 X^0}{\partial z^2} + g'(X^0)X^1\frac{\partial X^0}{\partial z}\,\mathrm{d}z \\
&= \int_{\mathbb{R}} X^1 \Big(\nabla {r^0}^{\mathrm{T}} P\nabla r^0 \frac{\partial}{\partial z}\frac{\partial^2 X^0}{\partial z^2} + g'(X^0)\frac{\partial X^0}{\partial z}\Big)\,\mathrm{d}z = 0.
\end{aligned}$$

By using this relation, we directly deduce from the multiplication of equation (5.8) by $\frac{\partial X^0}{\partial z}$ and integration that

$$\begin{aligned}
&\Big(\alpha\frac{\partial r^0}{\partial t} - \operatorname{div}(P\nabla r^0)\Big)\int_{\mathbb{R}} |\frac{\partial X^0}{\partial z}|^2\,\mathrm{d}z \\
&- \int_{\mathbb{R}} 2\frac{\partial^2 X^0}{\partial z^2}\nabla {r^1}^{\mathrm{T}} P\nabla r^0\frac{\partial X^0}{\partial z}\,\mathrm{d}z - \int_{\mathbb{R}} 2\sum_{l=1}^{2}\frac{\partial^2 X^0}{\partial z\partial s_l}\nabla {s_l}^{0\mathrm{T}} P\nabla r^0\frac{\partial X^0}{\partial z}\,\mathrm{d}z \\
&= \beta\vartheta^0\int_{\mathbb{R}}\frac{\partial X^0}{\partial z}\,\mathrm{d}z.
\end{aligned} \tag{5.10}$$

6. The Sharp Interface Model

We note that (see [1]) the surface tension is given by

$$\sigma = \int_{\mathbb{R}} |\frac{\partial X^0}{\partial z}|^2\,\mathrm{d}z.$$

Furthermore, the mean curvature of $\Gamma^0(t)$ is given by $\kappa^0 = \Delta r^0$. Hence, $\overline{\kappa} := \operatorname{div}(P\nabla r^0)$, which equals κ^0 in the case $P = I$, is related to the mean curvature. From the relation (5.6), we deduce $\int_{\mathbb{R}} \frac{\partial X^0}{\partial z}\,\mathrm{d}z = 2$, and we can thus rewrite equation (5.10) as

$$\begin{aligned}
&(-\alpha V - \overline{\kappa})\sigma - \int_{\mathbb{R}} 2\frac{\partial^2 X^0}{\partial z^2}\nabla {r^1}^{\mathrm{T}} P\nabla r^0\frac{\partial X^0}{\partial z}\,\mathrm{d}z \\
&- \int_{\mathbb{R}} 2\sum_{l=1}^{2}\frac{\partial^2 X^0}{\partial z\partial s_l}\nabla {s_l}^{0\mathrm{T}} P\nabla r^0\frac{\partial X^0}{\partial z}\,\mathrm{d}z \\
&= 2\beta\vartheta^0.
\end{aligned} \tag{6.1}$$

We collect the terms that would vanish in the derivation if $P = I$ as

$$\text{additional} := -\int_{\mathbb{R}} 2\frac{\partial^2 X^0}{\partial z^2}\nabla {r^1}^{\mathrm{T}} P\nabla r^0\frac{\partial X^0}{\partial z}\,\mathrm{d}z - \int_{\mathbb{R}} 2\sum_{l=1}^{2}\frac{\partial^2 X^0}{\partial z\partial s_l}\nabla {s_l}^{0\mathrm{T}} P\nabla r^0\frac{\partial X^0}{\partial z}\,\mathrm{d}z.$$

By recalling that ϑ^0 does not depend on z and by applying the matching condition (5.4), we deduce

$$\tilde{\theta}^0(t,\Gamma^0_\pm) = \frac{(-\alpha V - \overline{\kappa})\sigma}{2\beta} + \frac{\text{additional}}{2\beta}$$

and, thus,

$$\theta^0(t,x) = \frac{(-\alpha V - \overline{\kappa})\sigma}{2\beta} + \frac{\text{additional}}{2\beta} \quad \text{on } \Gamma^0(t).$$

This relation and the identities (4.2), (4.6), and (5.7) now yield the sharp interface model

$$\begin{gathered}\rho_{\mathrm{s}} {u^0}' - \operatorname{div}(P^{\mathrm{s}}\nabla u^0) + \kappa_{RI}(u^0 - \theta^0) = 0 \quad \text{in } S\times\Omega,\\ \rho_{\mathrm{p}} {\theta^0}' - \operatorname{div}(P^{\mathrm{p}}\nabla \theta^0) + \kappa_{RI}(\theta^0 - u^0) = 0 \quad \text{for } t\in S,\ x\in\Omega_l(t)\cup\Omega_s(t),\\ \nabla {r^0}^{\mathrm{T}} P^{\mathrm{p}} \nabla r^0 \big[\frac{\partial\theta^0}{\partial\vec{n}}\big]_{\Gamma^0_\pm} = -\lambda V \quad \text{for } t\in S,\ x\in\Gamma^0(t)\end{gathered}$$

with

$$\theta^0 = \frac{(-\alpha V - \overline{\kappa})\sigma}{2\beta} + \frac{\text{additional}}{2\beta} \text{ for } t\in S,\ x\in\Gamma^0(t),$$

which is of similar structure as the Stefan problem with surface tension and kinetic undercooling, compare to [1].

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Martin Höpker

Center for Industrial Mathematics, University of Bremen, Postfach 33 04 40, 28334 Bremen, Germany

E-mail address: hoepker@math.uni-bremen.de