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v odbore doktorandského štúdia:
9.1.9 Aplikovaná matematika

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v študijnom odbore 9.1.9 Aplikovaná matematika

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1 Introduction

The solidification of fluids is an integral part of many natural and industrial processes. Among typical examples is the formation of snowflakes and icicles in winter or the sea ice in polar areas. The phase-change processes play an important role also in material engineering during production of new materials such as metal castings and semiconductors. From the point of applications in material engineering, an important class of problems is that of solidification of multi-component systems (alloys).

It is a well known phenomenon that a material solidifying from an alloy usually has a different composition than the original system. For example, the ice growing from sea water is almost pure. The way in which the liquid material solidifies can affect the quality of the final product. A typical example is the appearance of structural defects, called freckles, during solidification of metal alloys (see Fowler 1985). To control the quality of solidified products, it is necessary to understand the coupling between fluid flow and solidification involved.

A mathematical model of diffusion-driven solidification of a binary alloy cooled below was studied by Worster (1986) as an extension of the classical Stefan problem for a single component system. The interface between the solid and liquid phases, characterised by the local conservation of heat and solute, was assumed planar. The rate of solidification in the model was controlled by the diffusive transport of solute away from the interface. Analytical self-similar solutions were found, with square-root time growth of the interface. Since the diffusion of solute is typically much slower that the diffusion of heat, a region of so-called constitutional supercooling often forms ahead of the solid/liquid interface, where the temperature of the liquid phase is below the local liquidus (freezing) temperature. Under such conditions a planar solid/liquid interface may become morphologically unstable, thus giving rise to the formation of highly convoluted structures, called dendrites. As a result, a so-called mushy layer forms, which is a region between the solid and liquid phases with a complicated microstructure. From the macroscopic point of view, the mushy layer is a reactive porous medium whose permeability changes in space and time upon the internal solidification/melting of its dendrites. Worster (1986) developed a model of a mushy layer, based on the local conservation of heat and solute, as an extension of the model with planar solid/liquid interface. The mushy layer was separated from the solid and liquid regions by planar interfaces with square-root time growth. The mathematical model was dimensional, with a large number of physical parameters — he assumed that the solid and liquid phases had different thermal properties. Therefore, the nonlinear, free-boundary problem governing the mushy layer could not be solved explicitly but only numerically via the shooting method. Gewecke & Schulze (2011*b*) assumed the equal thermal properties of the solid and liquid phases, along with the negligible latent-heat release. These assumption allowed them to find explicit self-similar solutions to the governing equations.

The self-similar form of solutions derived by Worster (1986) and Gewecke & Schulze (2011*b*) was a consequence of the semi-infinity of the solidifying system in the vertical direction, i.e. the direction perpendicular to the planar interfaces. Gewecke & Schulze (2011*a*) studied the dynamics of a mushy layer in a vertically-bounded region. Due

to the finite extent of the solidifying system, they could not use the self-similar approach. However, due to the hyperbolic character of the equation governing the liquid fraction in the mushy layer, they were able to study the problem via the method of characteristics. The main finding was that the mush/liquid interface retreated in a finite time in case when the solute diffusion was not neglected.

An experimental configuration in which the interface is stationary and that is also common in material engineering is the one in which a cooled horizontal boundary (substrate) is moving at a constant speed in horizontal direction in an imposed vertical temperature gradient (continuous strip and spin casting). There are two main features that distinguish such a configuration from those with a stationary cooled boundary or those of directional solidification: (*i*) the solidifying interface is not planar; (*ii*) there is a strong two-dimensional flow in the liquid phase. Such a configuration was previously addressed as a local approximation of spin casting (see the review by Steen & Karcher 1997). Löfgren & Åkerstedt (2001) studied the initial solidification of a pure liquid-metal film flow over a moving boundary. The problem of a steady two-dimensional boundary-layer flow of a binary alloy over a moving substrate was studied by Löfgren (2001). He obtained self-similar solutions for the velocity, temperature and solute concentration fields in the limit of small Prandtl number, which is typical of liquid metal flows. The interface was shown to have a square-root growth in the horizontal direction. The self-similar analysis was facilitated by the assumption of semi-infinite domain in vertical direction and that of small interfacial slope so that boundary-layer reduction was possible. An extension of the problem to include a mushy region was considered by Cheung, Shiah & Tangthieng (2002) and by Cheung & Tangthieng (2003). The mushy layer consisted of two separate layers: a packing region, with solid phase moving with the substrate, and a dispersed region, where solid phase was free to move with the fluid. The self-similar solutions were found numerically. However, the relationship between the local liquid fraction and temperature was prescribed through the lever rule, not by the local conservation of solute as by Worster (1986).

2 Goals of the thesis

The aim of this thesis is to combine the approach of Löfgren (2001) with that of Worster (1986) in order to formulate the problem studied by Cheung *et al.* (2002), such that the local liquid fraction will be given by the local conservation of solute. Unlike Cheung *et al.* (2002), we shall consider a simplified situation with the mushy layer consisting only of the packing region. Our task will be to find closed-form self-similar solutions to the governing equations and, using these solutions, study how the forced boundary layer flow influences the main physical characteristics of the mushy layer — the local liquid fraction and the positions of solid/mush and mush/liquid interfaces.

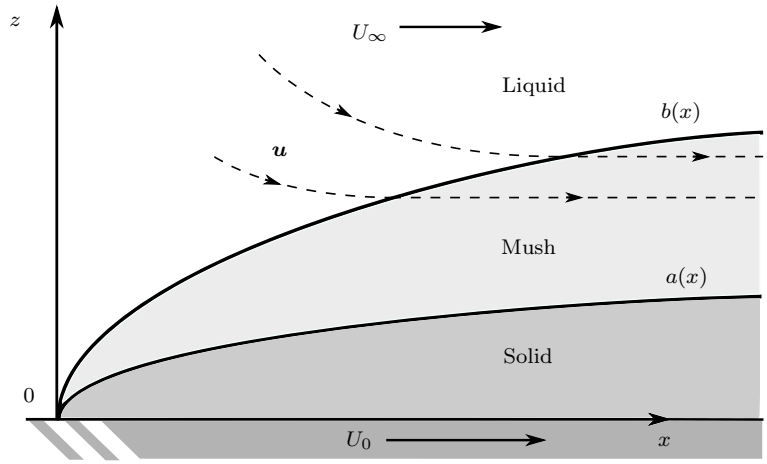

Figure 3.1: A definition sketch for the problem of solidification of a binary alloy over a horizontally moving boundary. A semi-infinite region $x > 0$, $z > 0$ is filled with a binary alloy of far-field solute concentration C_∞ and temperature T_∞ (for $z \to \infty$, x fixed). The cooled lower boundary lies in the plane $z = 0$ and is moving in horizontal direction at a constant speed U_0. The temperature of the cooled boundary is maintained at a value T_0. The stationary solid/mush and mush/liquid interfaces are located at $z = a(x)$ and $z = b(x)$.

3 Mathematical formulation

We consider a steady-state solidification of a binary alloy over a cooled plate $z = 0$, moving horizontally at constant speed $U_0 > 0$. The temperature of the moving plate is maintained at a value T_0 that is above the eutectic temperature T_E and below the liquidus temperature $T_L(C_\infty)$ corresponding to the far-field solute concentration C_∞ at $z \to \infty$. The far-field temperature in the liquid is T_∞. The binary alloy occupies the region $x > 0$, $z > 0$. The experimental setting of the present problem is the same as that by Löfgren (2001); a new feature in the present analysis is the presence of a steady mushy layer separated from the solid and liquid phases by interfaces located at $z = a(x)$ and $z = b(x)$, respectively. A definition sketch for the problem under consideration is depicted in figure 3.1. We denote by χ the local liquid fraction in the mushy layer.

3.1 Dimensional governing equations in the mushy layer

The speed of the material points embedded in the dendrites is

$$\boldsymbol{v} = U_0 \boldsymbol{k}, \tag{3.1}$$

while both interfaces are stationary. We define $\boldsymbol{k} = (1, 0)$.

We adopt the following assumptions to simplify the physical problem and to enable us to seek the solutions in a self-similar form:

i) We ignore the gravity as we do not assume any convective motions in the mush and liquid regions.

ii) We assume that there is no pressure gradient in the interstitial liquid of the mush.

3.1.1 Flow field in the mushy layer

The above assumptions imply that there is no flow relative to the dendrites, so the flow field $\boldsymbol{u}$ is given as

$$\boldsymbol{u} \equiv \boldsymbol{v} \tag{3.2}$$

and the streamlines are parallel to the x-axis (see figure 3.1). Moreover, (3.2) implies that the incompressibility is automatically satisfied.

3.1.2 Temperature and concentration fields in the mushy layer

The governing equation describing the temperature in the mushy layer is

$$U_0 \frac{\partial T}{\partial x} = \kappa \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial z^2} \right) - U_0 \frac{L}{C_P} \frac{\partial \chi}{\partial x}, \tag{3.3}$$

and the governing equation describing the concentration field is

$$U_0 \frac{\partial}{\partial x} (\chi C) = D \left[\frac{\partial}{\partial x} \left(\chi \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial z} \left(\chi \frac{\partial C}{\partial z} \right) \right]. \tag{3.4}$$

3.1.3 Liquidus relationship

We consider local thermodynamic equilibrium, given by a linear liquidus relationship of the following form

$$T = T_L(C) \equiv T_0 - \hat{\Gamma}(C - C_0), \tag{3.5}$$

where $\hat{\Gamma} > 0$ is the liquidus slope and C_0 is such that $T_0 = T_L(C_0)$. The corresponding phase diagram, along with the all relevant physical quantities, is depicted in figure 3.2.

3.1.4 Conditions at the interfaces

We denote by $\mathrm{D}a/\mathrm{D}t = -\boldsymbol{v} \cdot \boldsymbol{n}_a$ and $\mathrm{D}b/\mathrm{D}t = -\boldsymbol{v} \cdot \boldsymbol{n}_b$ the local velocities of the solid material elements relative to the (stationary) solid/mush and mush/liquid interfaces. We denote by $\boldsymbol{n}$ the outward unit vector normal to the interface. Then the conservation of heat and solute at the mush/liquid interface, respectively, take the following form

$$\rho L (1 - \chi_{b^-}) \frac{\mathrm{D}b}{\mathrm{D}t} = (k \boldsymbol{\nabla} T|_{b^-} - k \boldsymbol{\nabla} T|_{b^+}) \cdot \boldsymbol{n}_b, \tag{3.6a}$$

$$C_b (1 - \chi_{b^-}) \frac{\mathrm{D}b}{\mathrm{D}t} = D(\chi_{b^-} \boldsymbol{\nabla} C|_{b^-} - \boldsymbol{\nabla} C|_{b^+}) \cdot \boldsymbol{n}_b. \tag{3.6b}$$

and that at the solid/mush interface become

$$\rho L \chi_{a^+} \frac{\mathrm{D}a}{\mathrm{D}t} = (k \boldsymbol{\nabla} T|_{a^-} - k \boldsymbol{\nabla} T|_{a^+}) \cdot \boldsymbol{n}_a, \tag{3.7a}$$

$$C_{a^+} \chi_{a^+} \frac{\mathrm{D}b}{\mathrm{D}t} = -D \chi_{a^+} \boldsymbol{n}_a \cdot \boldsymbol{\nabla} C|_{a^+}. \tag{3.7b}$$

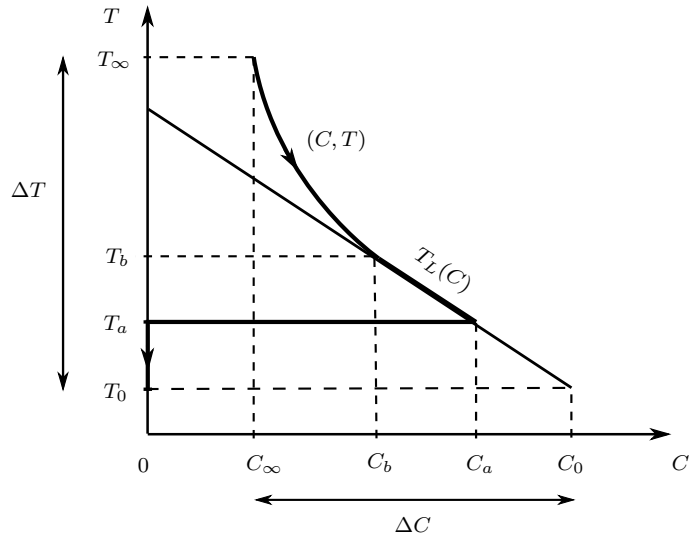

Figure 3.2: Approximate binary phase diagram for a system with a mushy layer, used in our thesis. For the description of particular symbols, see text. Shown is also a typical trajectory (C, T) of a solidifying system (solid lines with arrows).

3.1.5 Governing equations in the solid phase

The temperature field in the solid phase is governed by a stationary advection-diffusion equation of the following form

$$\boldsymbol{v} \cdot \boldsymbol{\nabla} T = \kappa \nabla^2 T, \tag{3.8}$$

or, equivalently,

$$U_0 \frac{\partial T}{\partial x} = \kappa \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial z^2} \right). \tag{3.9}$$

The advective term results from the horizontal advection of heat caused by the pulling of the substrate (and hence the whole solid phase) at the constant speed U_0 in the x-direction.

3.1.6 Governing equations in the liquid phase

The temperature and concentration fields in the liquid phase are governed by the stationary advection-diffusion equations

$$\boldsymbol{u} \cdot \boldsymbol{\nabla} T = \kappa \nabla^2 T, \tag{3.10}$$

$$\boldsymbol{u} \cdot \boldsymbol{\nabla} C = D \nabla^2 C. \tag{3.11}$$

The stationary, Navier-Stokes equations for the velocity field $\boldsymbol{u}$ are

$$(\boldsymbol{u} \cdot \boldsymbol{\nabla})\boldsymbol{u} = -\frac{1}{\rho} \boldsymbol{\nabla} P + \nu \nabla^2 \boldsymbol{u}, \tag{3.12}$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0, \tag{3.13}$$

where ν is the kinematic viscosity.

3.1.7 Boundary conditions

The boundary conditions imposed at the moving substrate, the mush/liquid interface and that at the far-field are

$$z = 0: \quad T = T_0, \tag{3.14a}$$
$$z = b: \quad u = U_0,\ v = 0, \tag{3.14b,c}$$
$$z \to \infty: \quad T \to T_\infty,\ C \to C_\infty, \tag{3.14d,e}$$
$$u \to U_\infty. \tag{3.14f}$$

The conditions (3.14b,c) impose the continuity of both the normal and tangential mass fluxes across the mush/liquid interface.

3.2 Dimensionless formulation

To render the governing equations dimensionless, we scale the velocities with U_0 and lengths with κ/U_0. In the rest of the thesis we will denote the dimensionless quantities by the same symbols as the dimensional ones. We define the dimensionless temperature and concentration, respectively, by

$$\theta = \frac{T - T_0}{\Delta T}, \quad \text{and} \quad \Theta = \frac{C_0 - C}{\Delta C}, \tag{3.15}$$

where

$$\Delta T = T_\infty - T_0, \quad \text{and} \quad \Delta C = C_0 - C_\infty. \tag{3.16}$$

Note that θ and Θ may vary from 0 to 1.

3.2.1 Mushy layer

The dimensionless governing equations in the mushy layer are

$$\frac{\partial \theta}{\partial x} = \frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial z^2} - \mathscr{S}\frac{\partial \chi}{\partial x}, \tag{3.17a}$$
$$(\Theta - \mathscr{C})\frac{\partial \chi}{\partial x} + \chi\frac{\partial \Theta}{\partial x} = \varepsilon\left[\frac{\partial}{\partial x}\left(\chi\frac{\partial \Theta}{\partial x}\right) + \frac{\partial}{\partial z}\left(\chi\frac{\partial \Theta}{\partial z}\right)\right], \tag{3.17b}$$
$$\theta = \theta_L(\Theta) \equiv \Gamma\Theta. \tag{3.17c}$$

The dimensionless groups appearing in the above equations are the inverse Lewis number ε, the Stefan number $\mathscr{S}$, the concentration ratio $\mathscr{C}$ and the dimensionless liquidus slope Γ, defined respectively by

$$\varepsilon = \frac{D}{\kappa}, \quad \mathscr{S} = \frac{L}{C_p \Delta T}, \quad \mathscr{C} = \frac{C_0}{\Delta C}, \quad \Gamma = \hat{\Gamma}\frac{\Delta C}{\Delta T}. \tag{3.18a–d}$$

Note that the effective range of $\mathscr{C}$ is $(1, \infty)$ and that of Γ is $(0, 1)$.

3.3 Boundary-layer reduction and self-similar formulation

Our goal is to examine self-similar solutions to the problem just stated, with the dimensionless interfaces having a square-root growth of the form

$$a(x) = 2\lambda_a x^{1/2}, \quad b(x) = 2\lambda_b x^{1/2}, \tag{3.18a,b}$$

where λ_a and λ_b are unknown positive constants. We shall consider a self-similar variable ζ, defined by

$$\zeta = \frac{z}{2x^{1/2}}. \tag{3.19}$$

However, the system of partial differential equations hitherto presented does not admit a self-similar solution involving the variable ζ. To facilitate the self-similar analysis, we consider the limit

$$x \to \infty, \quad z/x^{1/2} = O(1), \tag{3.20}$$

so that $\boldsymbol{n}_a$, $\boldsymbol{n}_b \sim \boldsymbol{k}$ to the leading order. The physical motivation for such limit is that the horizontal gradients of temperature and concentration are small relative to the gradients in vertical direction – a procedure that is typical of boundary layer analyses in fluid dynamics (see, for example, Schlichting 1979). In the limit (3.20), a self-consistent boundary-layer approximation of the governing dimensionless equations and the interface conditions can be made formally via the following re-scaling

$$(x, z) \mapsto (l\hat{x}, l^{1/2}\hat{z}), \tag{3.21}$$

using a fictitious dimensionless scale l, taking the limit $l \to \infty$ with $\hat{x} = O(1)$, $\hat{z} = O(1)$, collecting the leading order terms and then returning back to the original variables x and z. Below we state the reduced system of governing equations and the corresponding conditions at the interfaces.

Mushy layer

$$\frac{\partial \theta}{\partial x} = \frac{\partial^2 \theta}{\partial z^2} - \mathscr{S}\frac{\partial \chi}{\partial x}, \tag{3.22a}$$

$$(\Theta - \mathscr{C})\frac{\partial \chi}{\partial x} + \chi\frac{\partial \Theta}{\partial x} = \varepsilon\frac{\partial}{\partial z}\left(\chi\frac{\partial \Theta}{\partial z}\right), \tag{3.22b}$$

$$\theta = \Gamma\Theta. \tag{3.22c}$$

Liquid phase

$$u\frac{\partial \theta}{\partial x} + v\frac{\partial \theta}{\partial z} = \frac{\partial^2 \theta}{\partial z^2}, \tag{3.23a}$$

$$u\frac{\partial \Theta}{\partial x} + v\frac{\partial \Theta}{\partial z} = \varepsilon\frac{\partial^2 \Theta}{\partial z^2}, \tag{3.23b}$$

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial z} = Pr\frac{\partial^2 u}{\partial z^2}, \tag{3.24a}$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial z} = 0. \tag{3.24b}$$

where $Pr \equiv \nu/\kappa$ is the dimensionless Prandtl number.

Solid phase

$$\frac{\partial \theta}{\partial x} = \frac{\partial^2 \theta}{\partial z^2} \tag{3.25}$$

Mush/liquid interface

$$\mathscr{S}(1-\chi_{b^-})\frac{\mathrm{d}b}{\mathrm{d}x} = \left.\frac{\partial \theta}{\partial z}\right|_{b^-} - \left.\frac{\partial \theta}{\partial z}\right|_{b^+}, \tag{3.26a}$$

$$(\mathscr{C}-\Theta_b)(1-\chi_{b^-})\frac{\mathrm{d}b}{\mathrm{d}x} = \varepsilon\left(\left.\frac{\partial \Theta}{\partial z}\right|_{b^+} - \chi_{b^-}\left.\frac{\partial \Theta}{\partial z}\right|_{b^-}\right). \tag{3.26b}$$

Solid/mush interface

$$\mathscr{S}\chi_{a^+}\frac{\mathrm{d}a}{\mathrm{d}x} = \left.\frac{\partial \theta}{\partial z}\right|_{a^-} - \left.\frac{\partial \theta}{\partial z}\right|_{a^+}, \tag{3.27a}$$

$$(\mathscr{C}-\Theta_a)\chi_{a^+}\frac{\mathrm{d}a}{\mathrm{d}x} = \varepsilon\chi_{a^+}\left.\frac{\partial \Theta}{\partial z}\right|_{a^+}. \tag{3.27b}$$

4 Results

4.1 Velocity, temperature and concentration fields in the liquid phase

We consider the asymptotic limit of small Prandtl number, since this is the situation typical of liquid metal alloys. The velocity field can be obtained as

$$u = f', \tag{4.1a}$$

$$v = \frac{1}{x^{1/2}}(\zeta f' - f), \tag{4.1b}$$

where f is the solution of the third-order differential equation

$$Pr\, f''' + 2ff'' = 0, \tag{4.2}$$

subject to boundary conditions

$$\zeta = \lambda_b: \quad f = \lambda_b, \tag{4.3a}$$

$$f' = 1, \tag{4.3b}$$

$$\zeta \to \infty: \quad f' \to \mathscr{U}, \tag{4.3c}$$

where $\mathscr{U} = U_\infty/U_0$ is the velocity ratio. The asymptotic solution, found via the method of matched asymptotic expansions, reads

$$f(\zeta; Pr) \sim \lambda_b(1-\mathscr{U}) + \mathscr{U}\zeta + Pr\frac{1-\mathscr{U}}{2\lambda_b}\left[1-\exp\left(-2\lambda_b\frac{\zeta-\lambda_b}{Pr}\right)\right] \tag{4.3c}$$

as $Pr \to 0$.

4.2 Temperature and concentration fields

The temperature field is given as

$$\theta(\zeta) \sim 1 + (\theta_b - 1)\frac{\operatorname{erfc}\left[\mathscr{U}^{1/2}(\zeta - \lambda_b) + \mathscr{U}^{-1/2}\Lambda(\lambda_b)\right]}{\operatorname{erfc}\left[\mathscr{U}^{-1/2}\Lambda(\lambda_b)\right]}, \quad \zeta > \lambda_b, \tag{4.4}$$

where

$$\Lambda(\lambda_b) \equiv \lambda_b + Pr\frac{1 - \mathscr{U}}{2\lambda_b} \tag{4.5}$$

and θ_b is a part of the solution.

$$\Theta(\zeta) \sim 1 + (\Theta_b - 1)\frac{\operatorname{erfc}\left[(\mathscr{U}/\varepsilon)^{1/2}(\zeta - \lambda_b) + (\mathscr{U}\varepsilon)^{-1/2}\Lambda(\lambda_b)\right]}{\operatorname{erfc}\left[(\mathscr{U}\varepsilon)^{-1/2}\Lambda(\lambda_b)\right]}, \quad \zeta > \lambda_b, \tag{4.6}$$

with Θ_b being a part of the solution.

4.3 Temperature field in the solid phase

The temperature field in the solid phase reads

$$\theta = \theta_a\frac{\operatorname{erf}(\zeta)}{\operatorname{erf}(\lambda_a)}, \quad \zeta < \lambda_a. \tag{4.7}$$

4.4 Situation with solid/liquid interface

In case when there is no mushy layer in the system, the solid phase is separated from the liquid one by the interface at $\zeta = \lambda_h$, where λ_h is a root of

$$\Gamma\left[\lambda_h\frac{F[\Lambda(\lambda_h)/\mathscr{U}^{1/2}]}{G(\lambda_h)} + \Lambda(\lambda_h)\right]\Theta_h - \Lambda(\lambda_h) - \mathscr{S}\lambda_h F\left[\frac{\Lambda(\lambda_h)}{\mathscr{U}^{1/2}}\right] = 0, \tag{4.8}$$

with

$$F(\lambda) = \pi^{1/2}\lambda\,\mathrm{e}^{\lambda^2}\operatorname{erfc}(\lambda). \tag{4.9}$$

We found that in the limit $\mathscr{U} \to 0$, the following asymptotic approximation holds

$$\lambda_h \sim \varepsilon^{1/2}F_{\mathrm{inv}}(\mathscr{C}^{-1})\mathscr{U}^{1/2}, \quad \mathscr{U} \to 0, \tag{4.10}$$

provided $Pr \ll \mathscr{U} \ll 1$.

To see how small $\mathscr{U}$ affects the temperature and concentration fields, we approximate the leading-order forms (i.e. we set $Pr = 0$) of the temperature and concentration fields for $\mathscr{U} \to 0$ and $\zeta = O(1)$. For the temperature we obtain

$$\theta \sim \frac{2\varepsilon^{1/2}F_{\mathrm{inv}}(\mathscr{C}^{-1})}{F[\varepsilon^{1/2}F_{\mathrm{inv}}(\mathscr{C}^{-1})]}(\zeta - \lambda_h)\mathscr{U}^{1/2} \tag{4.11}$$

and for the concentration

$$\Theta \sim 2\varepsilon^{-1/2}\mathscr{C}F_{\mathrm{inv}}(\mathscr{C}^{-1})(\zeta - \lambda_h)\mathscr{U}^{1/2}. \tag{4.12}$$

Moreover, we see from (4.3c) that small $\mathscr{U}$ modifies the viscous boundary layer such that its effective thickness is $O(Pr/\mathscr{U}^{1/2}) \ll O(1/\mathscr{U}^{1/2})$. Therefore, the asymptotic condition $Pr \ll \mathscr{U} \ll 1$ can be interpreted such that Pr and $\mathscr{U}$ must be small in such a way that the viscous boundary layer resides within the concentration one. As a result, the effect of the viscous boundary layer on the transport of heat and solute is negligible in the leading order (cf. Löfgren 2001) and it is through the velocity ratio that the flow affects the solidification. Therefore, the concentration and thermal fields together with the growth rate λ_h can well be approximated by their leading-order forms in Pr.

4.5 Mushy layer with solute diffusion

In case when the mushy layer is present in the system, the liquid fraction is governed by the following differential equation

$$\frac{\chi'}{\chi} = \frac{2\zeta\Theta' + \varepsilon\Theta''}{2\zeta(\mathscr{C} - \Theta) - \varepsilon\Theta'}, \tag{4.13}$$

with the solution in the form

$$\chi = \chi_{b^-} \exp\left(- \int_{\zeta}^{\lambda_b} \frac{2s\Theta' + \varepsilon\Theta''}{2s(\mathscr{C} - \Theta) - \varepsilon\Theta'} \, \mathrm{d}s \right). \tag{4.14}$$

The governing equation for the temperature field in the mushy layer becomes

$$\theta'' + 2\zeta\theta' = -2\mathscr{S}\zeta\chi', \tag{4.15}$$

which, due to the liquidus relationship, also determines the governing equation for the concentration field

$$\Theta'' + 2\zeta\Theta' = -2\frac{\mathscr{S}}{\Gamma}\zeta\chi'. \tag{4.16}$$

The condition (3.27a), expressing the conservation of heat at the solid/mush interface, transforms via (3.19) into the following form

$$2\mathscr{S}\chi_{a^+}\lambda_a = \theta'_{a^-} - \theta'_{a^+}. \tag{4.17}$$

The conservation of solute, expressed by (3.27b), transforms into the equation

$$\left[2\lambda_a(\mathscr{C} - \Theta_a) - \varepsilon\Theta'_{a^+}\right]\chi_{a^+} = 0. \tag{4.18}$$

The conservation of heat, given by (3.26a), transforms to

$$2\mathscr{S}(1 - \chi_{b^-})\lambda_b = \theta'_{b^-} - \theta'_{b^+}. \tag{4.19}$$

At this point we take into account the condition of marginal equilibrium, proposed by Worster (1986). In the present scaling, this condition can be expressed as

$$\theta'_{b^+} = \Gamma\Theta'_{b^+}. \tag{4.20}$$

Using (4.20), we can rewrite (4.19) as

$$2\mathscr{S}(1-\chi_{b^-})\lambda_b = \Gamma\left(\Theta'_{b^-} - \Theta'_{b^+}\right). \tag{4.21}$$

The conservation of solute (3.26b) takes the form

$$2(\mathscr{C}-\Theta_b)(1-\chi_{b^-})\lambda_b = \varepsilon\left(\Theta'_{b^+} - \chi_{b^-}\Theta'_{b^-}\right). \tag{4.22}$$

We found that χ obeys the following integral equation

$$\left[2\zeta(\mathscr{C}-\Theta) - \varepsilon\Theta'\right]\chi = 2\int_{\lambda_a}^{\zeta}(\mathscr{C}-\Theta)\chi\,\mathrm{d}s, \tag{4.23}$$

that can be used to show that $\chi_{b^-} = 1$ and that the concentration gradient is continuous across the mush/liquid interface. We also showed that

$$2\lambda_a(\mathscr{C}-\Theta_a) - \varepsilon\Theta'_{a^+} = 0. \tag{4.24}$$

regardless the value of Stefan number. This result extends that of Gewecke & Schulze (2011a) to the case when Stefan number is non-zero. For $\mathscr{S} > 0$, showed that the gradient of liquid fraction at the solid/mush interface, χ'_{a^+}, is bounded, while the numerical calculations suggest that it is unbounded when $\mathscr{S} = 0$. The boundedness of the liquid-fraction gradient for positive Stefan numbers is a direct consequence of the coupling between the liquid fraction and the temperature field, represented by the heat equation with the source term due to the local latent-heat release. Therefore, the singularity of the liquid-fraction gradient turns out to be the consequence of the negligible Stefan number.

When $\mathscr{S} = 0$, the governing equations in the mushy layer can be solved explicitly. The temperature field in the mushy layer reads

$$\theta = \theta_a\frac{\mathrm{erf}(\zeta)}{\mathrm{erf}(\lambda_a)}, \tag{4.25}$$

and the concentration fields

$$\Theta = \Theta_a\frac{\mathrm{erf}(\zeta)}{\mathrm{erf}(\lambda_a)}, \quad \lambda_a \le \zeta \le \lambda_b. \tag{4.26}$$

Due to the condition (4.24) the integral has a singularity at $\zeta = \lambda_a^+$, which complicates the numerical integration in the vicinity of this point. We use the integral equation (4.23) to show that $\chi_{a^+} = 0$ when Stefan number is zero.

The explicit solution can be used to derive, using the conservation laws at the solid/mush interface, the following nonlinear algebraic equation for the growth constant λ_a.

$$\left[\Theta_b - \mathscr{C}\frac{\mathrm{erf}(\lambda_b)}{\mathrm{erf}(\lambda_a)}\right]G(\lambda_a) + \varepsilon\Theta_b = 0. \tag{4.27}$$

The algebraic equation for the growth constant λ_b, derived from the conservation laws at the mush/liquid interfaces, reads

$$\varepsilon\lambda_b F\left[\frac{\Lambda(\lambda_b)}{(\varepsilon\mathscr{U})^{1/2}}\right] - \Gamma\lambda_b F\left[\frac{\Lambda(\lambda_b)}{\mathscr{U}^{1/2}}\right] + (1-\Gamma)\Lambda(\lambda_b)G(\lambda_b) = 0. \tag{4.28}$$

Since the diffusion of heat is typically more rapid than that of solute, the inverse Lewis number, ε, is small. However, the growth of the mushy layer is governed primarily by the thermal balances at the interfaces. Therefore the advance of the mush/liquid interface is not restricted by the diffusion of solute away from the interface. As a result, the mushy layer exists even when the diffusion of solute is negligible, with no solid phase present in the system — such situation corresponds to setting $\varepsilon = 0$ (cf. Gewecke & Schulze 2011*a* for the case of a mushy layer on a finite domain). We shall discuss the case $\varepsilon = 0$ in the next chapter. However, the limit $\varepsilon \to 0$ is singular in the liquid phase, the concentration field having the boundary layer of thickness $O(\varepsilon^{1/2})$.

In the limit $\varepsilon \to 0$, we derived the following approximation

$$\lambda_a = \frac{\varepsilon}{\pi^{1/2}\mathscr{C}\,\mathrm{erf}(\lambda_b)} + O(\varepsilon^2) \quad \text{as} \quad \varepsilon \to 0. \tag{4.29}$$

Thus the growth of the solid phase is governed by diffusion of solution and the growth of the mushy layer is governed by the diffusion of heat, since $\lambda_b = O(1)$ as $\varepsilon \to 0$.

The asymptotic limits $\varepsilon \to 0$ and $\mathscr{U} \to 0$ are interchangeable and therefore regular. To the leading order in Pr, ε and $\mathscr{U}$, the algebraic equation for the growth constant λ_b is as takes the following form

$$G(\lambda_b) = \frac{\Gamma}{1-\Gamma} \tag{4.30}$$

Moreover, $\theta_b \to \Gamma$ as $\varepsilon \to 0$. Therefore Γ is the quantity that dominantly controls the thickness of the mushy layer.

4.6 Mushy layer with no solute diffusion - global conservation model

When the solute diffusion is neglected, we can model the conservation of solute in the mushy layer in two different ways: locally and globally. The models hitherto discussed were all local as they assumed the conservation of solute within infinitesimal volume elements. While the local conservation of solute is possible in both cases of zero and non-zero solute diffusion, the global model is applicable only under the assumption of zero solute diffusion. The idea of the global conservation model was first introduced by Huppert & Worster (1985). Another useful reference can be found in the review by Huppert (1993). Thompson, Huppert & Worster (2003) developed a global conservation model for diffusion-controlled growth of a ternary alloy under the assumption that the temperature profile in the mushy layer was linear.

In out thesis, we use the global approach to investigate the effect of the forced boundary-layer flow in the liquid phase, represented by the dimensionless numbers Pr and $\mathscr{U}$, on the characteristics of the mushy layer. Then we discuss the local conservation model and its relation to the global one. Though the local model with negligible solute diffusion has already been studied by other authors, new in our investigation are the dimensionless scalings and the explicit relation between the liquid fractions in the local and global models in case when Stefan number is negligible.

In the global conservation model, we require that the average bulk concentration (per unit length in the horizontal direction) within the mushy layer is equal to that in the liquid phase, C_∞[1], and that the volume fraction $\chi = \chi_{\rm glob}$ is uniform, which yields

$$\frac{1}{\lambda_b}\int_0^{\lambda_b}(\mathscr{C}-\Theta)\chi_{\rm glob}\,{\rm d}\zeta = \mathscr{C}-1. \tag{4.31}$$

The temperature and concentration fields, respectively, are given as

$$\theta(\zeta) = \theta_b\frac{{\rm erf}(\zeta)}{{\rm erf}(\lambda_b)}, \tag{4.32}$$

and

$$\Theta(\zeta) = \frac{{\rm erf}(\zeta)}{{\rm erf}(\lambda_b)}. \tag{4.33}$$

The liquid fraction can be expressed, using (4.31) and (4.33), as

$$\chi_{\rm glob} = \frac{\mathscr{C}-1}{\mathscr{C}-1+H(\lambda_b)}, \tag{4.34}$$

The Stefan condition at the mush/liquid interface reads

$$\mathscr{S}(1-\chi_{\rm glob})\frac{{\rm d}b}{{\rm d}x} = \left.\frac{\partial\theta}{\partial z}\right|_{b^-} - \left.\frac{\partial\theta}{\partial z}\right|_{b^+}. \tag{4.35}$$

Note that, unlike the local conservation model, in which $\chi_{b^-}=1$, in the global model the left hand-side of the Stefan condition is always nonzero when $\mathscr{S}>0$. Indeed, in the global model, the solidification occurs only at the interface and the global conservation forces the uniform volume fraction to be less than unity in the mush. Using (4.32), we can express the condition (4.35) as

$$\mathscr{U}^{1/2}\frac{{\rm e}^{\lambda_b^2}\,{\rm erf}(\lambda_b)}{{\rm e}^{\Lambda^2(\lambda_b)/\mathscr{U}}\,{\rm erfc}[\Lambda(\lambda_b)/\mathscr{U}^{1/2}]} = \frac{1}{1-\Gamma}\left[\Gamma+\mathscr{S}\frac{1-{\rm e}^{\lambda_b^2}}{\mathscr{C}-1+H(\lambda_b)}\right]. \tag{4.36}$$

To simplify the mathematical problem, we will consider the regular limit of negligible Stefan number. In this limit, the thickness of the mushy layer is independent of $\mathscr{C}$. Moreover, the concentration ratio affects the system only through the quantity $\chi_{\rm glob}$. Note that

$$\chi_{\rm glob} \to 1-\frac{1}{2\mathscr{C}-1} \quad \text{as} \quad \lambda_b\to 0, \tag{4.37}$$

which is the value obtained by Worster (2000) under the quasi-stationary approximation, in which the temperature profile in the mush could be well approximated by its steady form owing to the fact that the heat conduction was rapid compared to the rate of solidification. One way to ensure a slow solidification rate is to assume large values of Stefan number, resulting in a thin mushy layer. Though in the present

[1]The concentration of solute in the liquid phase is uniform when there is no solute diffusion; it is a direct consequence of the equations governing the concentration field in the liquid phase.

case we have $\mathscr{S} = 0$, the temperature profile in the mush can be treated as linear provided λ_b is small enough.

With $\mathscr{S} = 0$, the nonlinear equation for λ_b becomes

$$\mathit{\Gamma}\lambda_b F\left[\frac{\mathit{\Lambda}(\lambda_b)}{\mathscr{U}^{1/2}}\right] + (\mathit{\Gamma} - 1)\mathit{\Lambda}(\lambda_b)G(\lambda_b) = 0. \tag{4.38}$$

We can make further simplification by taking the regular limit $Pr \to 0$ in the above equation to obtain

$$\mathit{\Gamma} F\left(\frac{\lambda_b}{\mathscr{U}^{1/2}}\right) + (\mathit{\Gamma} - 1)\lambda_b G(\lambda_b) = 0. \tag{4.39}$$

It can be shown that $\lambda_b = O(1)$ as $\mathscr{U} \to 0$ such that (4.39) reduces to a simple equation

$$G(\lambda_b) = \frac{\mathit{\Gamma}}{1 - \mathit{\Gamma}} \quad \text{for} \quad \mathscr{S} = 0,\ Pr \to 0,\ \mathscr{U} \to 0, \tag{4.40}$$

which is the same as (4.30).

It is instructive to have a closer look at the definitions of dimensionless numbers $\mathscr{C}$ and $\mathit{\Gamma}$. It is straightforward to show that these numbers are, in fact, not independent, since

$$\mathscr{C}\mathit{\Gamma} = \frac{\hat{\mathit{\Gamma}} C_0}{\Delta T}. \tag{4.41}$$

The relation stated above will prove useful in the physical interpretation of different asymptotic limits.

$\mathscr{C} \to 1$ with $\mathit{\Gamma}$ fixed This limit is equivalent to $C_\infty \to 0$ so that the bulk composition in the system decreases to zero. Moreover, (4.34) implies that $\chi \to 0$: as the initial composition decreases, there is less solute to be rejected upon solidification and hence the growth of dendrites is enhanced.

$\mathscr{C} \to \infty$ with $\mathit{\Gamma}$ fixed This limit is equivalent to $C_\infty \to C_0$ with λ_b fixed. Moreover, (4.41) implies $\hat{\mathit{\Gamma}} C_0/\Delta T \sim \mathscr{C} \to \infty$ so that $\Delta T \to 0$ (recall that $\Delta T \equiv T_\infty - T_0$). Finally, (4.34) implies $\chi \to 1$: increasing the far-field concentration (and hence the bulk concentration in the mush) results in melting of dendrites. In order to keep the thickness (in terms of λ_b) of the mushy layer unaffected, we need to decrease the far-field temperature of the melt.

$\mathscr{C} \to \infty$ with $\mathscr{C}\mathit{\Gamma}$ fixed In this limit, $\mathit{\Gamma} \sim \mathscr{C}^{-1} \to 0$ with $\hat{\mathit{\Gamma}} C_0/\Delta T$ kept fixed. As in the limit with fixed $\mathit{\Gamma}$ discussed above, the liquid fraction tends to unity ($\chi \to 1$). However, (4.40) implies that $\lambda_b \to 0$. Thus, when $C_\infty \to C_0$ with C_0, ΔT and $\hat{\mathit{\Gamma}}$ kept fixed, the thickness of mushy layer decreases.

To include the effect of latent heat release when as $\mathscr{U} \to 0$, the equation (4.36) can be approximated, to leading order, as follows

$$G(\lambda_b)\left(1 + \frac{Pr}{2\lambda_b^2}\right) = \frac{1}{1 - \mathit{\Gamma}}\left[\mathit{\Gamma} + \mathscr{S}\frac{1 - \mathrm{e}^{\lambda_b^2}}{\mathscr{C} - 1 + H(\lambda_b)}\right]. \tag{4.42}$$

We found that the positive values of Stefan number result in finite values of λ_b as $\mathit{\Gamma} \to 1^-$.

4.7 Mushy layer with no solute diffusion – local conservation model

While in the global conservation model the absence of the solid phase in the system was assumed a priori, however, in the local model it is a direct consequence of the conservation of solute at the solid/mush interface.

In the local conservation model with zero solute diffusion, the bulk composition in the mushy layer is constant, i.e.

$$\frac{\partial}{\partial x}[(\mathscr{C}-\Theta)\chi]=0. \tag{4.43}$$

The above equation follows from (3.22b) by setting $\varepsilon=0$. The temperature field in the mushy layer is governed by

$$\frac{\partial\theta}{\partial x}=\frac{\partial^2\theta}{\partial z^2}-\mathscr{S}\frac{\partial\chi}{\partial x}. \tag{4.44}$$

However, since the limit $\mathscr{S}\to 0$ is regular, in what follows, we set $\mathscr{S}=0$ in order to derive explicit solutions. The governing equations in the liquid phase does not differ from those used in the global model, with homogenous concentration $\Theta\equiv 1$.

The value of liquid fraction at the interface can be deduced from the local conservation of solute at the interface

$$(\mathscr{C}-1)(1-\chi_{b^-})\frac{\mathrm{d}b}{\mathrm{d}x}=0, \tag{4.45}$$

so that

$$\chi_{b^-}=1 \tag{4.46}$$

is the only consistent solution. Thus the liquid fraction in the mush can be expressed as

$$\chi=\frac{\mathscr{C}-1}{\mathscr{C}-\Theta}. \tag{4.47}$$

The local conservation of solute at the solid/mush interface implies

$$(\mathscr{C}-\Theta_a)\chi_{a^+}\frac{\mathrm{d}a}{\mathrm{d}x}=0. \tag{4.48}$$

However, from (4.47) we have $\chi_{a^+}=(\mathscr{C}-1)/(\mathscr{C}-\Theta_a)$, which is nonzero since $\mathscr{C}>1$. Thus the only way to satisfy the above equation is to set $\mathrm{d}a/\mathrm{d}x=0$ so that

$$\lambda_a=0, \tag{4.49}$$

which implies that there is no solid in the system in case when the solute diffusion is neglected. Since $\Theta_0=0$, we obtain the liquid fraction at the bottom of the mushy layer

$$\chi_{0^+}=1-\frac{1}{\mathscr{C}}. \tag{4.50}$$

Note that χ_{0^+} is always positive even for positive values of Stefan number.

The temperature field in the mushy layer has the form

$$\theta = \Gamma \frac{\mathrm{erf}(\zeta)}{\mathrm{erf}(\lambda_b)} \tag{4.51}$$

and the concentration field

$$\Theta = \frac{\mathrm{erf}(\zeta)}{\mathrm{erf}(\lambda_b)}. \tag{4.52}$$

Recall that $\theta_b = \Gamma$ due to the liquidus relationship between the temperature and concentration fields and the fact that $\Theta_b = 1$.

Since we assume $\mathscr{S} = 0$, the Stefan condition at the mush/liquid interface implies the continuity of temperature gradient at this interface, as was also the case in the global conservation model. Using the explicit solutions derived above together with the solution for the temperature field in the liquid, the continuity of temperature gradient can be used to derive an algebraic equation for the growth constant λ_b in the following form

$$\Gamma \lambda_b F\left[\frac{\Lambda(\lambda_b)}{\mathscr{U}^{1/2}}\right] + (\Gamma - 1)\Lambda(\lambda_b)G(\lambda_b) = 0. \tag{4.53}$$

We obtained the equation that is the same as (4.38) that we derived for the global conservation model. However, this is not surprising since the only difference between the global and local models is in the liquid fractions in the mush. Particularly, the Stefan condition has the same mathematical expression in both models. When $\mathscr{S} = 0$, the liquid fractions does not enter the Stefan conditions as the left hand-sides of these conditions are zero. Thus we have shown that for zero Stefan number and for given values of Γ, $\mathscr{C}$, Pr and $\mathscr{U}$ the thickness of the mushy layer in the local conservation model is the same as that in the global one, as well as the temperature and concentration fields. Using this information, we can derive a relationship between the liquid fractions in the global and local models. Since λ_b and the concentration field in the global and local models are the same, we can combine (4.31) with (4.47) to obtain

$$\frac{1}{\lambda_b}\int_0^{\lambda_b} \frac{\mathrm{d}\zeta}{\chi} = \frac{1}{\chi_{\mathrm{glob}}}, \tag{4.54}$$

that is, the reciprocal liquid fraction in the global model is equal to the average reciprocal liquid fraction in the local model.

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Conferences, winter and summer schools

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- Algoritmy 2009 – Conference on Scientific Computing (15 - 20 March 2009, Vysoké Tatry, Podbanské, `http://www.math.sk/alg2009/`; presentation of a poster)
- Advanced Topics in Numerical and Computational Bifurcation Analysis (summer school, 13 - 19 June 2011, Copenhagen, Denmark)
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