International Journal of Thermal Sciences 48 (2009) 2013–2016

Contents lists available at ScienceDirect

International Journal of Thermal Sciences

journal homepage: www.elsevier.com/locate/ijts

Call for contributions to a numerical benchmark problem for 2D columnar solidification of binary alloys

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ARTICLE INFO

Article history:
Available online 26 August 2009

Keywords:
Benchmark
Solidification
Columnar growth
Binary mixture
Thermosolutal convection

ABSTRACT

This call describes a numerical comparison exercise for the simulation of ingot solidification of binary metallic alloys. Two main steps are proposed, which may be treated independently: 1. The simulation of the full solidification process. First a specified 'minimal' solidification model is used and the contributors are provided with the corresponding sets of equations. The objective is to verify the agreement of the numerical solutions obtained by different contributors. Then different physical solidification models may be compared to check the features that allow for the best possible prediction of the physical phenomena. 2. A separate preliminary exercise is also proposed to the contributors, only concerned with the convective problem in the absence of solidification, in conditions close to those met in solidification processes. Two problems are considered for the case of laminar natural convection: transient thermal convection for a pure liquid metal with a Prandtl number on the order of 10^{-2}, and double-diffusive convection in an enclosure for a liquid binary metallic mixture with a Prandtl number on the order of 10^{-2} and a Lewis number on the order of 10^4.

This call for contribution aims at proposing a set of comparison exercises for the sake of verification and validation of mathematical models and numerical codes concerned with ingot solidification of binary metallic alloys.

This exercise consists of two main steps, which may be treated independently.

1. The main phase concerns the simulation of the full solidification process, in two different stages:
   - A stage of verification [4]: comparison of the numerical results obtained by different codes using a specified «minimal» solidification model resulting from the volume averaging technique. The contributors are provided with the corresponding sets of equations and the objective is to verify the degree of agreement of the numerical solutions of the contributors.
   - A stage of validation: comparison of the different physical solidification models of the contributors. The objective of this stage is the best possible prediction of the physical phenomena. This exercise is closely linked to experiments that are being developed within the present project and it will be treated later.
2. A separate preliminary exercise is also proposed to the contributors, which deals only with the convective aspect of the problem in the absence of solidification, in conditions close to those met in solidification processes. Two problems are considered for the case of laminar natural convection:
   - Transient thermal convection for a pure liquid metal with a Prandtl number on the order of 10^{-2}, referring to the initial thermal transient period in a solidification process with initial liquid superheat,
   - Double-diffusive convection in an enclosure for a liquid binary metallic mixture with a Prandtl number on the order of 10^{-2} and a Lewis number on the order of 10^4, to simulate thermo-solutal convective flows in the bulk liquid zone during solidification.

The main features of the comparison exercise are described hereafter, but the complete details (problem description, system of equations, parameters, initial and boundary conditions, thermophysical properties and format of outputs) may be found on the

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doi:10.1016/j.ijthermalsci.2009.07.024

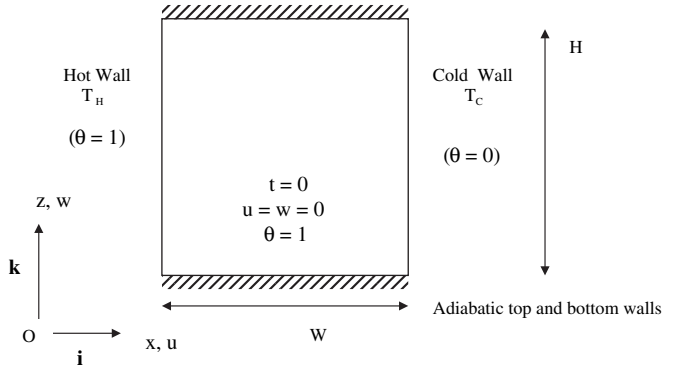

Fig. 1. Description of the thermal convection problem.

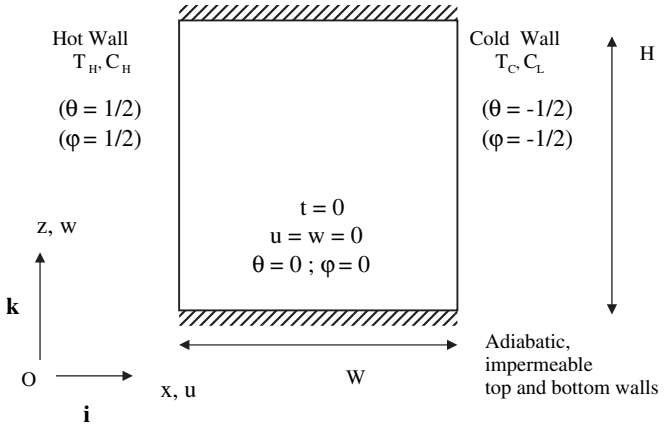

Fig. 2. Description of the thermo-solutal convection problem.

benchmark website: http://www.ijl.nancy-universite.fr/benchmark-solidification.

1. Preliminary exercise: natural convection

Given the complexity of the coupled heat and mass transfer model and of the physics involved in the simulation of solidification processes, it appears useful to draw the attention of contributors to the specific difficulties related to the solution of the fluid mechanics problem in those processes. In this exercise, two classes of problems are relevant to this situation:

1. The transient convective flow during initial heat extraction from the superheated liquid metal, characterized by a low Prandtl number;
2. The double-diffusive convection flow in the bulk liquid zone, driven by the thermal gradient and solute rejection/absorption at the front, characterized by very high Lewis numbers and low Prandtl numbers.

1.1. Transient natural convection

The first convection exercise consists in the simulation in transient thermal natural convection in a rectangular cavity, shown in Fig. 1. It is assumed that there is no solidification. A no-slip condition is assumed at all walls. The top and bottom walls are adiabatic and temperatures are imposed at the left and right walls. The fluid is initially at rest at the hot temperature T_H and at $t = 0$ the temperature of the right wall is set at the cold temperature T_C. The dimensionless parameters are listed below:

Dimensionless parameters		
Prandtl number	*Pr*	10^{-2}
Grashof number	*Gr*	5×10^7
Aspect ratio	*A*	1

The results are to be presented in dimensionless form. If contributors require dimensional variables, the reference variables provided on the website allow for the conversion of the results into a non-dimensional term for the sake of comparison.

1.2. Thermo-solutal convection

The second exercise consists in the simulation of cooperating thermo-solutal convection of a liquid binary metallic mixture in conditions representative of solidification. Again, it is assumed that there is no solidification. The top and bottom walls are adiabatic and no-slip. The left and right walls are no-slip. Different but uniform imposed temperatures and concentrations are applied at each vertical wall. The fluid is initially at rest at the mean temperature T_M and at the mean concentration C_M and at $t = 0$ the temperature of the left wall is set at the hot temperature T_H and its concentration at the high concentration C_H, while the right wall is set at the cold temperature T_C and the low concentration C_L (Fig. 2). These conditions are quite different from the solidification conditions, but the purpose is to characterize the double diffusive fields in such a cavity. The parameters are listed below:

Dimensionless parameters		
Prandtl number	*Pr*	10^{-2}
Lewis number	*Le*	10^4
Thermal Grashof number	*Gr*	5×10^6
Buoyancy ratio	*N*	5
Aspect ratio	*A*	1

The output variables to be provided and their format are specified on the website.

2. Benchmark: ingot solidification

2.1. The reference problem

The configuration chosen for the comparison exercise is a 2D ingot casting problem where heat is extracted from both vertical walls of a rectangular mold initially filled with a stagnant liquid binary metal at a uniform temperature and composition. Only few experimental results are available in the literature, and in order to

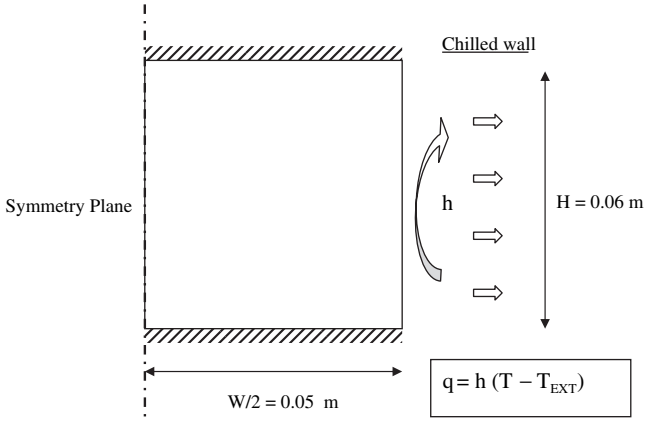

Fig. 3. Description of the solidification problem.

allow for a comparison with these experiments, a geometry similar to the experiments by Hebditch and Hunt [1] is retained. A similar experiment is being developed in the frame of the present project (description on the website).

We consider the solidification of a binary alloy in a 2D rectangular box of height $H = 0.060$ m and width $W = 0.100$ m. Initially, the cavity is filled with a stagnant liquid alloy at a uniform temperature T_O, equal to the liquidus temperature (T_{LIQ}), and of uniform nominal concentration C_O. At time $t = 0$, solidification is started by cooling the left and right walls of the enclosure through an external cooling fluid at a temperature (T_{EXT}) and a overall heat transfer coefficient h. The cooling is described by a Fourier-type boundary condition:

$$q = h(T - T_{EXT}).$$

The top and bottom walls of the cavity are thermally insulated and the symmetry of the problem allows for the definition of the computational domain sketched in Fig. 3.

After the onset of cooling a solid phase and a mushy layer grow from the cooled walls and convective motions driven by both thermal and solutal buoyancy occur in the liquid phase. A rigid and connected solid phase is assumed, which forms an isotropic porous mush in the phase change zone. No-slip conditions at the cavity walls are assumed.

2.2. Imposed model

The objective of this exercise is to test the ability of the different numerical methods and algorithms to agree on a solution and to produce a reference numerical solution of the given problem. The imposed "minimal" (i.e. simplified to the largest possible degree) model for solidification of a binary alloy is based on the following usual hypotheses:

- Laminar flow and constant viscosity μ_l.
- Solute diffusion in the liquid and solid at the macroscopic scale is neglected.
- The solid and liquid densities are equal and constant ($\rho_s = \rho_l = \rho_0$), except in the buoyancy term of the momentum conservation equation, where ρ linearly depends on temperature T and solute concentration C_l (Boussinesq approximation).
- Saturated mixture.
- Local thermodynamic equilibrium is assumed, with perfect solute diffusion in both phases (lever rule).
- The solid phase is assumed to be motionless.
- The mushy zone is an isotropic porous medium whose permeability K is defined by the Carman–Kozeny relation.

2.2.1. Hypotheses

Saturated medium

$$g_s + g_l = 1 \tag{1}$$

Fixed solid phase

$$v_s = 0 \tag{2}$$

Thermal expansion is neglected except in the buoyancy term

$$\rho_s = \rho_l = \rho = \text{cst} \tag{3}$$

(Consequence: mass fractions = volumetric fractions).

Thermal equilibrium between phases

$$T_s = T_l = T \tag{4}$$

Constant thermal conductivity

$$k_s = k_l = k = \text{cst} \tag{5}$$

Table 1
Physical properties of Pb-18% Sn and Sn-10% Pb.

Property	Symbol	Units	Pb-18% Sn	Sn-10% Pb
Specific heat	c_p	$J\,(kg\,K)^{-1}$	176	260
Thermal conductivity	k	$W\,(m\,K)^{-1}$	17.9	55.0
Reference density	ρ_o	$Kg\,m^{-3}$	9250	7000
Latent heat of fusion	L	$J\,kg^{-1}$	3.76×10^4	6.1×10^4
Liquid dynamic viscosity	μ_l	Pa s	1.10×10^{-3}	1.0×10^{-3}
Liquid thermal expansion coefficient	β_T	K^{-1}	1.16×10^{-4}	6.0×10^{-5}
Liquid solutal expansion coefficient	β_C	$(wt\%)^{-1}$	4.90×10^{-3}	-5.3×10^{-3}
Secondary dendrite arm spacing	λ_2	m	1.85×10^{-4}	65.0×10^{-6}
Melting point at $C = 0$	T_m	°C	327.5	232.0
Eutectic composition	C_e	wt%	61.911	38.1
Equilibrium partition coefficient	k_P		0.310	0.0656
Liquidus slope	m	$°C\,(wt\%)^{-1}$	−2.334	−1.286
Nominal concentration	C_o	wt%	18.0	10.0
Initial temperature	$T_0 = T_{LIQ}$	°C	285.488	219.14
Heat transfer coefficient	h	$W\,m^{-2}\,K^{-1}$	400	400
External temperature	T_{EXT}	°C	25	25

Constant heat capacity

$$c_{ps} = c_{pl} = c_p = \text{cst} \tag{6}$$

2.2.2. Conservation equations

The conservation equations result from volume averaging of local conservation equations (e.g. see [2,3]). Following the above assumptions[1]:

Notation

$$\begin{aligned} \mathbf{V} &= g_l \mathbf{v}_l \\ p &= p_l \end{aligned} \tag{7}$$

Liquid momentum

$$\nabla\cdot(\mu_l\nabla\mathbf{V}) - g_l\nabla p - \frac{\mu_l g_l}{K}\mathbf{V} + g_l\tilde{\rho}\mathbf{g} = \rho_0\frac{\partial\mathbf{V}}{\partial t} + \frac{\rho_0}{g_l}(\nabla\mathbf{V})\mathbf{V} \tag{8}$$

Mass

$$\nabla\cdot\mathbf{V} = 0 \tag{9}$$

Energy

$$\rho_0\frac{\partial\langle h\rangle}{\partial t} + \rho_0 c_p\nabla T\cdot\mathbf{V} - \nabla\cdot(k\nabla T) = 0 \tag{10}$$

Solute

$$\frac{\partial\langle C\rangle}{\partial t} + \nabla C_l\cdot\mathbf{V} = 0 \tag{11}$$

2.2.3. Additional relations[2]

Permeability of the mush

$$K = \frac{\lambda_2^2 g_l}{180\,(1-g_l)^2} \tag{12}$$

[1] Note that the mixture theory leads to a different equation for momentum conservation: $\nabla\cdot(\mu_l\nabla\mathbf{V}) - \nabla p - \frac{\mu_l}{K}\mathbf{V} + \tilde{\rho}\mathbf{g} = \rho_0(\frac{\partial\mathbf{V}}{\partial t} + (\nabla\mathbf{V})\mathbf{V})$.

[2] Note: on the thermodynamic equilibrium diagram of this alloy, the existence of a eutectic reaction at the temperature T_e, corresponding to the eutectic composition C_e ($T_e = T_m + mC_e$), is considered.

Density variation with temperature and composition

$$\tilde{\rho} = \rho_0(1 - \beta_T(T - T_0) - \beta_c(C_l - C_0)) \quad (13)$$

Enthalpies

$$\begin{aligned} h_s &= c_p T \\ h_l &= c_p T + L \\ \langle h \rangle &= c_p T + g_l L \end{aligned} \quad (14)$$

Microsegregation model (lever rule)

$$\begin{aligned} \langle C \rangle &= g_l C_l + g_s C_s = (g_l + k_P(1 - g_l))C_l \\ T &= T_m + mC_l \end{aligned} \quad (15)$$

2.2.4. Test cases

Two different situations are proposed for the comparison exercise:

1. Solidification of a binary Pb-18% Sn alloy
2. Solidification of a binary Sn-10% Pb alloy

The thermophysical properties of the two alloys are specified in Table 1. They are assumed to be constant. The parameters of the problem allow the assumption of laminar flow.

The output variables to be provided and their format are specified on the website.

Acknowledgement

This comparison exercise is proposed in the frame of French National Research Agency (ANR) under project ANR-07-BLAN-190.

References

[1] Hebditch D.J., Hunt J.D. (1974): Metallurgical Transactions 5, pp. 1557–1564.
[2] J. Ni, C. Beckermann, A volume-averaged two-phase model for transport phenomena during solidification, Metallurgical Transactions B 22 (1991) 349–361.
[3] M. Rappaz, M. Bellet, M. Deville, Numerical Modeling in Materials Science and Engineering, Springer Series in Computational Mathematics, Springer-Verlag, 2003, Chapter 5.
[4] P.J. Roache, Verification of codes and calculations, AIAA Journal 36 (5) (1998) 696–702.