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

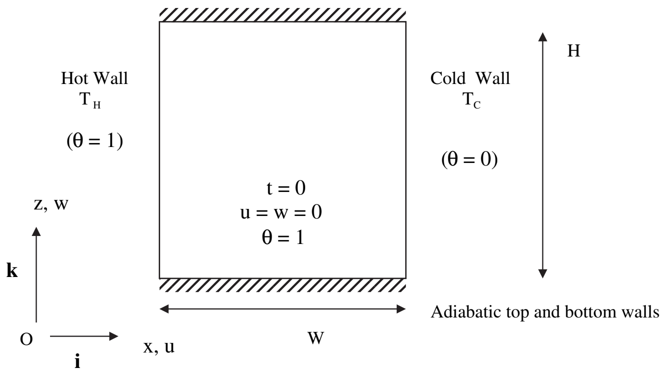


**Fig. 1.** Description of the thermal convection problem.

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* | $5 \times 10^7$ |
| 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:

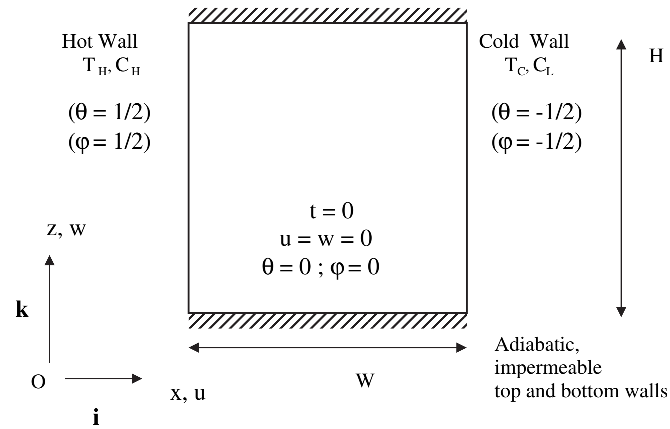


**Fig. 2.** Description of the thermo-solutal convection problem.

| Dimensionless parameters | | |
|---|---|---|
| Prandtl number | *Pr* | $10^{-2}$ |
| Lewis number | *Le* | $10^4$ |
| Thermal Grashof number | *Gr* | $5 \times 10^6$ |
| 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

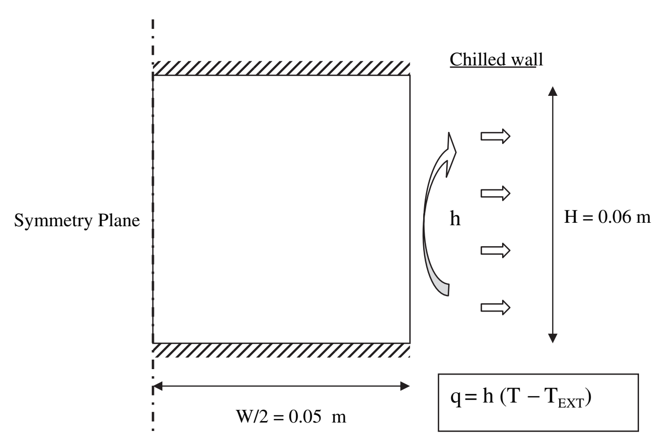


**Fig. 3.** Description of the solidification problem.