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NUMERICAL SIMULATION OF THE NATURAL CONVECTION IN A HORIZONTAL BRIDGMAN APPARATUS

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ABSTRACT

This work presents the numerical simulation of the natural convection with phase-change of succinonitrile (SCN) in a horizontal Bridgman apparatus. The analysis is carried out with two different numerical approaches: a thermally coupled temperature-based finite element formulation for generalized phase-change problems and a finite volume discretization using an enthalpy-porosity technique to account for the latent heat effect. Both numerical results are compared with the experimental data obtained from the literature.

RESUMEN

En este trabajo se presenta la simulación numérica de la convección natural con presencia de cambio de fase del material plástico SCN ("succinonitrile") en el dispositivo experimental conocido como test de Bridgman. El análisis se lleva a cabo mediante dos técnicas numéricas diferentes: una formulación de elementos finitos con un modelo basado en la temperatura para la descripción del cambio de fase y una formulación de volúmenes finitos que considera el efecto de cambio de fase mediante el método de la entalpía en el que la zona de interacción entre ambas fases se trata como un medio poroso. Los resultados obtenidos para la posición del frente de cambio de fase se comparan entre sí y con mediciones experimentales disponibles en la literatura.

1. INTRODUCTION

The modelling of natural convection in phase-change materials is particularly important in the analysis of engineering processes such as those present in casting industries where the correct evaluation of temperature evolutions and heat transfer conditions play a crucial role in the properties of the final products. Due to this, several efforts have been devoted in the last decades to the development of numerical formulations for the analysis of thermally coupled flows and, afterwards, to their experimental validation. The directional solidification of succinonitrile (SCN) in the Bridgman apparatus has been more recently proposed as a physical experiment to assess the reliability of different numerical simulations [1,2]. This plastic material is often used in crystal growth research owing to it mimics metal behaviour in a lower temperature range that makes it more proper to handle in practical experiments.
The aim of this work is to present a numerical analysis of the succinonitrile phase-change occurring in a horizontal Bridgman set-up. This thermally coupled flow problem is approached using the continuity, motion and energy equations. Their spatial discretization is obtained through two different fixed-mesh numerical techniques: a finite element (FEM) and a finite volume (FVM) methods. In the FEM framework, the weak form of the differential

equations is obtained via a generalized streamline operator technique together with a temperature-based model to account for the phase-change effects [3,4]. On the other hand, an enthalpy-porosity phase-change model is used in FVM approach [5,6].
The steady-state material response of SCN is analysed in the Bridgman test for a fixed position of the heating and cooling jackets (i.e., no-growth conditions). An isothermal phase-change and the Boussinesq approximation to describe the buoyancy effects are both assumed in the computations. Finally, the obtained interface front positions are compared with the experimental one reported in [1,2].

2. GOVERNING EQUATIONS AND DISCRETIZED FORMULATIONS

Natural convection with phase-change effects can be described by the well-known incompressible thermally coupled Navier-Stokes equations for a Newtonian fluid written as [1-6]:

- continuity equation

$$\nabla \cdot v = 0 \qquad \text{in } \Omega_l \times Y \qquad (1)$$

- equation of motion

$$\rho \dot{v} + \rho (v \cdot \nabla) v + \nabla p - \nabla \cdot (2\mu \in) = \rho b \quad \text{in } \Omega_l \times Y \qquad (2)$$

- energy equation

$$\rho \left(c + L \frac{\partial f_{pc}}{\partial T} \right) \left(\dot{T} + \nabla T \cdot v \right) = \nabla \cdot (k \nabla T) \quad \text{in } \Omega \times Y \qquad (3)$$

together with adequate boundary and initial conditions, where Ω is an open-bounded domain (subscript l indicates liquid phase) with smooth boundary Γ, Y is the time interval of interest ($t \in Y$), v is the velocity vector, p is the pressure, ρ is the fluid density, μ is the dynamic viscosity, ∇ is the gradient operator, ε is the rate of deformation tensor defined as $\varepsilon = \frac{1}{2}(\nabla_x v + v_x \nabla)$ and b is the specific body force including the Boussinesq approximation $b = g[1-\alpha(T-T_{REF})]$ with g being the gravity vector, α the volumetric thermal expansion coefficient, T the temperature and the subscript REF denoting a reference value. Moreover, c is the specific heat capacity, L is the specific latent heat, k is the conductivity coefficient and fpc is the phase-change function defined for a pure material as: fpc=H(T-Tm), where H is the Heaviside function and Tm is the melting temperature. The energy equation can also be written in terms of the enthalpy variable [5,6] with the following definition for its material time derivative: Dh/Dt=c DT/Dt + L Dfpc/Dt. Equations (1) and (2) are solved in Ω_l while equation (3) is computed in the whole domain Ω considering a null velocity field in the solid phase.
In the context of FEM, the integral form of equations (1-3) is obtained using a generalized streamline operator technique providing stabilized numerical results for the primitive variables of the problem: velocity, pressure and temperature. The latent heat effects are described using a temperature-based formulation avoiding the use of any regularization in the phase-change function definition. The strongly coupled system of equations is solved with a consecutive-converged-iterative staggered algorithm. The time integration is performed via an Euler backward scheme. Full details of this methodology can be found in [3,4].
The FVM considered in this work uses a second order approximation in both space and time discretizations. In this formulation, an enthalpy-porosity technique is applied to describe the

phase-change effects. Thus, the domain is decomposed in three regions, namely the solid and liquid phases and, moreover, the solid/liquid transition (mushy zone) defined with a small regularization parameter arbitrarily chosen as a percentage of Tm; see [5,6] and references therein for further details.

3. ANALISYS OF THE HORIZONTAL BRIDGMAN TEST

The low-temperature horizontal Bridgman test is an attractive experimental procedure aimed at promoting directional solidification or melting of materials occupying a differentially heated ampoule. In the experiments conducted and reported in [1,2], the ampoule was made of borosilicate glass and it was square in cross-section with dimensions 6mm inside, 8mm outside and 150mm length. The ampoule was filled under vacuum with SCN which has a very low conductivity and melting temperature. For the zero growth-rate conditions analysed, phase-change was induced by controlling the temperature of the outer boundary of the ampoule via fixed in position heating and cooling jackets such that the gap between them allowed observations of the solid-liquid interface and seed particles for velocimetry. These jackets were maintained at temperatures above and below the melting point of SCN. The thermo-physical properties of SCN and glass are listed in Table 1. The outside ampoule temperatures were measured longitudinally along different locations where temperature and position measurement accuracies were estimated to be approximately $\pm 1^{\circ}C$ and ± 0.5mm respectively. In the experiments, the temperature difference between the two jackets was $63^{\circ}C$ approximately. Further details of this experimental procedure are described in [1,2].

Table 1: thermo-physical properties of SCN and glass of the ampoule.

Property	Succinonitrile (SCN)	Glass
Density [kg/m^3]	980 (liquid) 1016 (solid)	2300
Specific heat [J/kg °C]	2000 (liquid) 1955 (solid)	753.5
Conductivity [W/m °C]	0.223 (liquid) 0.225 (solid)	1.2
Thermal expansion coeff. [1/°C]	0.00081 (liquid)	
Dynamic viscosity [kg/ms]	0.00256 (liquid)	
Melting temperature [°C]	58.09	
Specific latent heat [J/kg]	46500	

For simplicity, two-dimensional conditions are assumed in the present numerical analysis since, according to [1], the flow pattern and heat transfer conditions are not strongly affected by three-dimensional effects. The computational domain is restricted to the central length of the ampoule due to the experimentally observed temperature variations outside this region were found to be negligible [1,2]. Central lengths of 80mm and 52.5mm have been respectively considered for the FEM and FVM simulations. Steady-state conditions are only analysed considering impermeable boundaries of the liquid-filled region and temperature profiles on the outer surface of the glass walls derived from the experiments [1,2]. Non-uniform 60x20 and 60x40 meshes have been respectively chosen for FEM and FVM computations.

The computed and experimental steady-state solid-liquid interface positions are plotted in Figure 1. The distorted shape of the interface clearly indicates the significant influence of natural convection in the liquid on the phase-change front. An overall good agreement between the numerical predictions and the experiments can be appreciated. It should be noted

that the discrepancies observed in these curves are smaller than the error associated with the location of the interface position (±0.5mm). Moreover, these numerical results are also quantitatively concordant to those reported in [1].

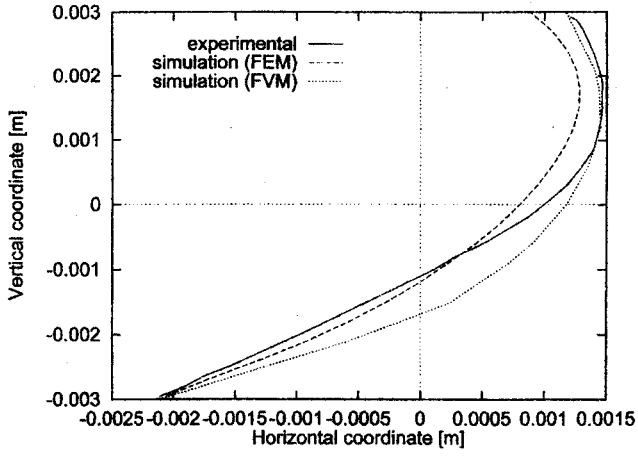
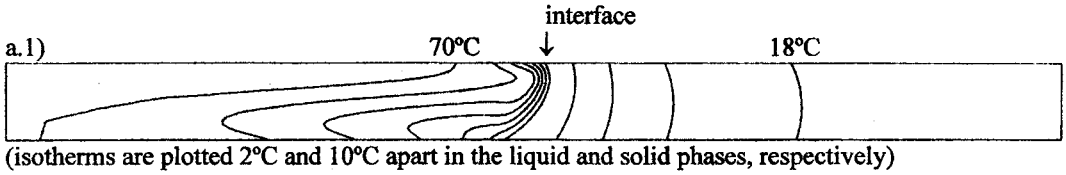
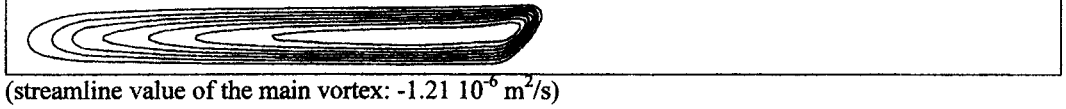


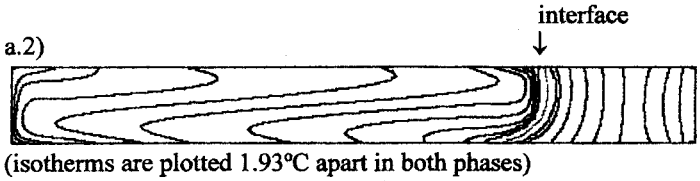
Figure 1: steady-state solid-liquid interface position.



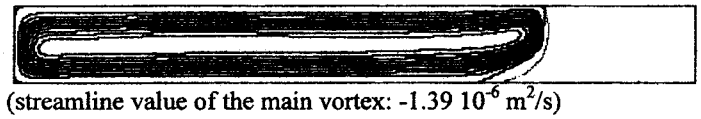
(isotherms are plotted 2°C and 10°C apart in the liquid and solid phases, respectively)



(streamline value of the main vortex: -1.21 10^{-6} m^2/s)



(isotherms are plotted 1.93°C apart in both phases)



(streamline value of the main vortex: -1.39 10^{-6} m^2/s)

Figure 2: steady-state a) isotherms and b) streamlines computed with 1) FEM and 2) FVM.

Figure 2 shows the computed steady-state isotherm and streamline contours obtained with FEM and FVM. Once again, the isotherms are highly deformed by the convection currents in the liquid phase. This distortion can be seen to propagate also into the solid. The streamlines show the development of a main vortex. The higher velocities computed with FEM are found to take place in the region near the interface while the FVM solution depicts a more uniform distribution. In general, the predicted velocity modulus are in the range of the experimental values derived from approximate observations of particle tracks. The numerical maximum velocity located at the mid-height of the ampoule in the vicinity of the phase-change front is 1.24mm/s which reasonably agrees with the experimental measurement of 1.64mm/s.

4. CONCLUSIONS

The analysis of the succinonitrile phase-change phenomenon that takes place in a horizontal Bridgman test has been presented using two different numerical approaches. In this problem, both methods have provided very similar results. In particular, the predicted steady-state interface front positions fit very well the experimental profile. The temperature and velocity fields obtained in this work are in accordance with those of previously published simulations and in qualitative good agreement with approximate experimental observations.

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ANÁLISIS DE FLUJOS CON SUPERFICIE LIBRE EN PROBLEMAS INDUSTRIALES

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RESUMEN

Durante la colada continua de acero en la industria siderúrgica, el metal fundido debe circular por una serie de recipientes antes de solidificar y tomar su forma final. Las características del flujo en estos recipientes influyen sobre la calidad del producto, lo que motiva el estudio de la fluidodinámica del proceso. En este trabajo se analiza numéricamente el flujo en el interior de un molde de planchones y de una cuchara, con particular énfasis en el comportamiento de la superficie libre.
Se utiliza un modelo de flujo turbulento incompresible que se resuelve mediante la técnica de elementos finitos. La condición de incompresibilidad es impuesta por penalización y la turbulencia es modelada con el modelo de longitud de mezcla o con el modelo k-ε. El método de las pseudoconcentraciones es empleado para estimar la posición de la superficie libre.
El modelo numérico fue validado con mediciones tomadas de la literatura realizadas en modelos de agua de un molde de planchones. Finalmente, se presentan resultados de la formación del vórtice en el proceso de vaciado de una cuchara.

ABSTRACT

During the continuous casting of steel, in steel industry, the molten metal circulates through a series of vessels before solidifying and taking its final shape. The characteristics of the flow inside these vessels affect the quality of the final product. This motivates the study of the fluid dynamics of the continuous casting process. In this work the flow inside a slab mold and inside a ladle is analyzed with particular attention to the free surface behaviour.
A turbulent incompressible fluid is considered. The finite element method is used to solve the equations. Incompressibility condition is imposed by penalization and the turbulence is modeled by the mixing length model or the k-ε model. Free surface position is estimated by the pseudoconcentration technique.
The numerical model was validated with measurements taken from literature performed on a water model of a slabs mold. Finally, results from the vortex formation during a ladle drainage are presented.

INTRODUCCIÓN

En la industria siderúrgica actual, la mayor parte de la producción de acero tiene lugar a través del proceso de colada continua. En este proceso, el acero líquido generado en el horno es transportado en un recipiente llamado cuchara hasta un repartidor o tundish donde vierte su contenido. El tundish, a su