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Numerical simulation of convection in a horizontal bridgman apparatus

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Abstract

The aim of this work is to present a numerical simulation of the directional solidification and melting of succinonitrile SCN (SCN: $NC(CH_2)_2CN$) in a horizontal Bridgman apparatus. Succinonitrile is a plastic material with low melting point and a thermal response similar to that of many metals. Three kinds of experiments were considered in order to analyze the material phase change behavior inside this furnace: "no growth", "solidification" and "melting" cases. For all cases, the results showed a good qualitative agreement between the experimental and simulated shapes of steady state solid – liquid interfaces. In particular, a remarkable fitting has been achieved for the "no growth" case. For both the "solidification" and "melting" cases, however, some discrepancies, attributed to the major influence of convection on the curvature of the solid – liquid interface produced by the movement of the external jackets, have been found.

Keywords: numerical simulation, phase change, convection, Bridgman apparatus, succinonitrile.

Resumen

El objetivo de este trabajo es presentar una simulación numérica de la solidificación direccional y fusión del succinonitrilo SCN (SCN: $NC(CH_2)_2CN$) dentro de un aparato u horno horizontal Bridgman. El succinonitrilo es un material plástico que presenta un bajo punto de fusión y una respuesta térmica similar a la mayoría de los metales. Se consideraron tres tipos de experimentos para analizar el comportamiento del cambio de fase en este material dentro del horno: "no crecimiento", "solidificación" y "fusión". Para los tres casos analizados, los resultados mostraron un buen ajuste cualitativo entre la forma experimental y numérica de la interfase sólido – líquido estacionaria. En particular, se obtuvo un ajuste preciso en el caso de "no crecimiento". Sin embargo, se observaron algunas discrepancias en los casos de "solidificación" y "fusión", atribuibles a la influencia mayor de la convección sobre la curvatura de la interfase sólido – líquido, producida por el movimiento longitudinal de las camisas externas del horno.

Palabras claves: simulación numérica, cambio de fase, convección, aparato Bridgman, succinonitrilo.

1. Introduction

Solidification and melting of materials are two of the most important processes in the manufacturing of products, reason why is important its study. Aerospace, automotive, optical and electronic industry have been requiring during the last decades components with less quantity of defects and high levels of homogeneity. Experimental research in processes which involve liquid metals is very complicated due to factors like opacity, reactivity and high operational temperatures. Besides, accurate experimental determination in the shape of the solid – liquid interface is very difficult to obtain. Directional solidification using Bridgman apparatus is widely used for this purpose [1,2]. The Bridgman apparatus allows to control solidification and melting of materials by means of movement of its external jackets with extremely low rates (e.g., within the range of 1 to 100 μm/s) in order to obtain a phase change under nearly equilibrium conditions. To reduce these difficulties and increase the precision in the measurements, transparent polymeric materials, such as succinonitrile, are typically used due to its low melting point which facilitates its handling.

The analysis of this process is carried out in this work by using a finite element methodology (FEM) aimed at simulating the physical phenomena that experience the material inside the apparatus. The numerical analysis of three specific experiments reported in the literature [2] is performed. In the first experiment, called the "no growth" case, the jackets kept fixed till reaching the steady state of the solid and liquid phases inside the glass tube. For the second experiment, the "solidification" case, the phase transformation is controlled externally by means of heating and cooling jackets, thus with its movement from right to left, the solid – the liquid interface moves with them and the solidification of SCN occurs. For the thirst and last experiment, the "melting" case, the jackets move through the opposite direction producing the phase change or melting of the solid. In all the experiments, heat transfer is produced through convection and radiation between the glass tube and jackets of the apparatus. The numerical results obtained for the position of the phase change interface are compared with available experimental measurements.

2. Governing equations

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:

- **Continuity equation:**

$$\nabla \cdot \nu = 0 \quad in\ \Omega_l \times Y \qquad (1)$$

- **Motion equation:**

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

- **Energy equation:**

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

together with adequate boundary and initial conditions, Ω is an open bounded domain (subscript l indicates liquid phase) with smooth boundary Γ, Y is the time interval of interest ($t \in Y$), ν 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 $\varepsilon = 1/2(\nabla \cdot \nu + \nu \cdot \nabla)$ and b is the specific body force including the Boussinesq approximation $b = g[1-a(T-T_{REF})]$ with g being the gravity vector, a 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: $fpc=H(T-T_m)$, where H is the Heaviside function and T_m is the melting temperature. Equations (1) and (2) were solved in Ω_l while equation (3) was 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) to (3) was 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 were described using a temperature based formulation avoiding the use of any regularization in the phase change function definition. The strongly coupled system of equations was solved with a consecutive-converged-iterative staggered algorithm. The time integration was performed via an Euler backward scheme. Full details of this methodology can be found in [3,4].

3. Experimental

The low-temperature horizontal Bridgman test is an attractive experimental procedure aimed at promoting directional solidification or melting of materials occupying a differentially heated glass tube in the apparatus; see Figure 1. In the experiments conducted and reported in [2], the glass tube was made of borosilicate with a square cross-section of 6 mm inside, 8 mm outside and 150 mm length; see Figure 2. The glass tube was filled under vacuum with SCN, which has a very low thermal conductivity and melting temperature. The thermo-physical properties of SCN and borosilicate are listed in Table 1. This apparatus has two types of external jackets; heating and cooling jackets which according to their movements, a purely heat transfer, solidification or melting processes can be achieved. The "no growth", "solidification" and "melting" cases are separately described below.
For the three cases, the difference in temperature between the heating and cooling jackets was approximately 63 °C with values above and below the melting point of SCN (58.09 °C), respectively. Heat transfer between external jackets and glass tube was realized by means of the "gap" or little space generated between them, producing a longitudinal distribution of temperature on the surface of the tube. For the "no growth" case, the initial percentage of solid was 50% in volume; while for "solidification" and "melting" cases were 33 and 67%, respectively. The outside glass tube temperatures were measured longitudinally along different locations, where temperature and position measurement accuracies were estimated to be approximately ± 1 °C and ± 0.5 mm, respectively. All experiments were carried out until steady state, being stopped when percentages of solid reached 67% and 33% for "solidification" and "melting" cases, respectively. Further details of this experimental procedure are described in [2].

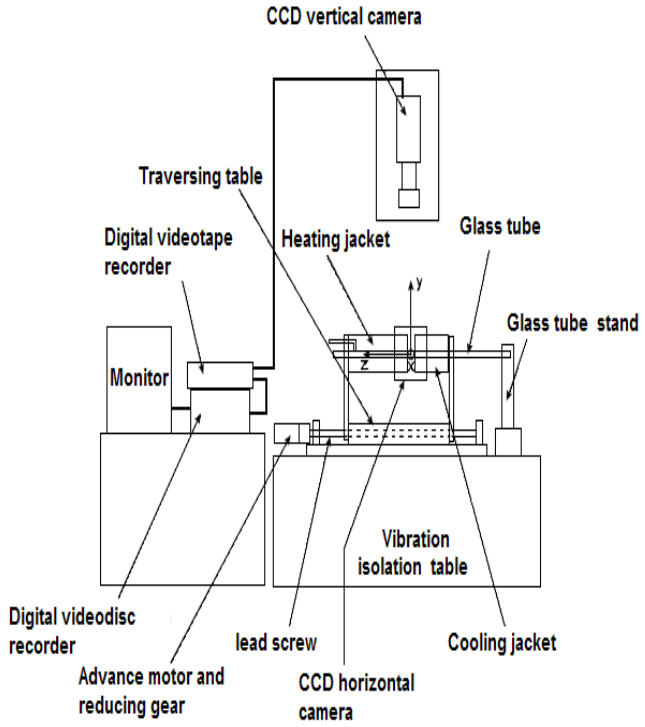

Figure 1: Bridgman apparatus.

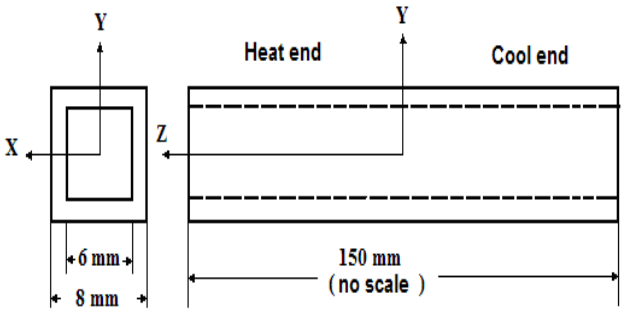

Figure 2: Geometric description of the glass tube used in the Bridgman apparatus.

Table 1: Thermo-physical properties of SCN and borosilicate.

Property	Succinonitrile (SCN)	Borosilicate
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 coefficient [1/°C]	0.00081 (liquid)	
Dynamic viscosity [kg/m·s]	0.00256 (liquid)	
Melting temperature [°C]	58.09	
Specific latent heat [J/kg]	46500	

3.1 "No growth" case

For the zero growth-rate conditions analyzed, phase change was induced by controlling the temperature of the outer boundary of the glass tube via fixing the position of heating and cooling jackets, such that the "gap" between them allowed to see observations of the solid-liquid interface and seed particles for velocimetry; see Figure 3. Boundary conditions for this case are given in Figure 4.

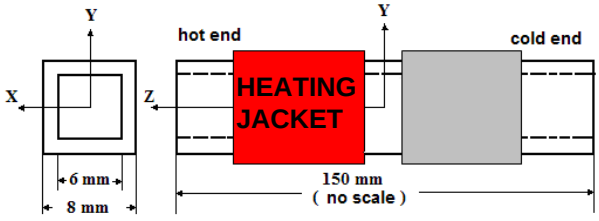

Figure 3: Scheme for the "no growth" case.

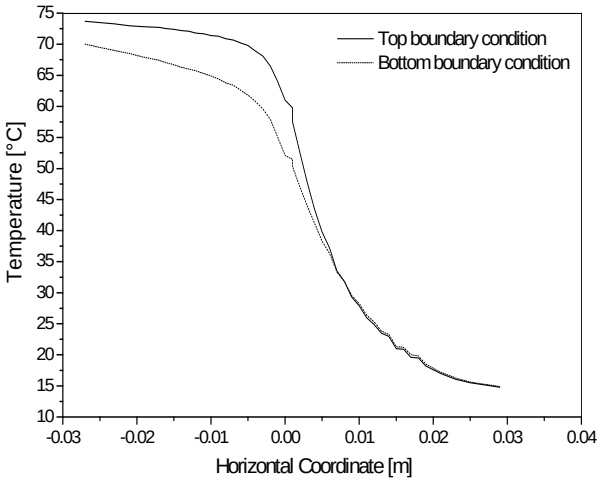

Figure 4: Boundary conditions for the "no growth" case.

3.2 "Solidification" case

Solidification was induced by controlling the temperature of the outside of the glass tube through the heating and cooling jackets together with positioning the glass tube, or moving them through the apparatus by means of the translation mechanism as well; see Figure 5. As the heating and cooling jackets moved from right to left over the fixed glass tube, the solid-liquid interface moved with them and solidification of the SCN occurred. Boundary conditions for this case are given in Figure 6.

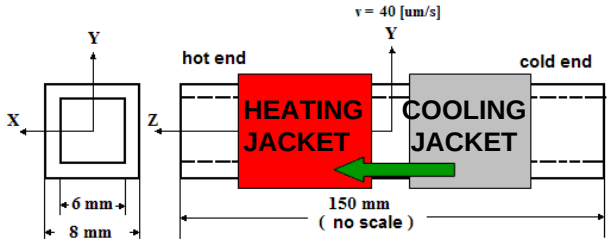

Figure 5: Scheme for the "solidification" case.

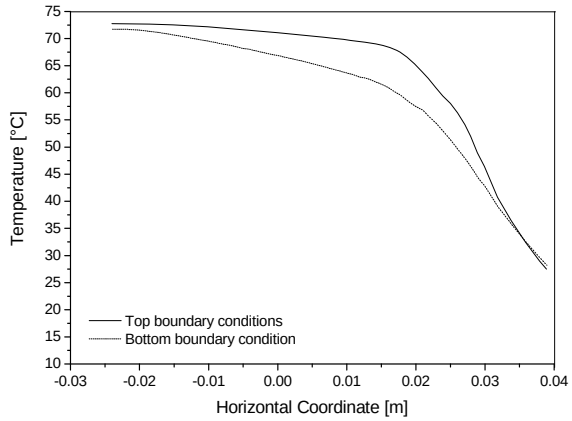

Figure 6: Boundary conditions for the "solidification" case.

3.3 "Melting" case

The mechanism used in this case is the same than solidification, but melting was achieved by moving the jackets in the reverse direction, i.e., from left to right; see Figure 7. Boundary conditions for this case are given in Figure 8.

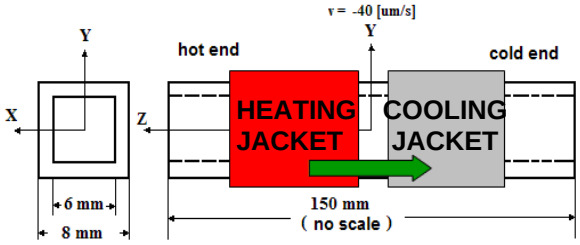

Figure 7: Scheme for the "melting" case.

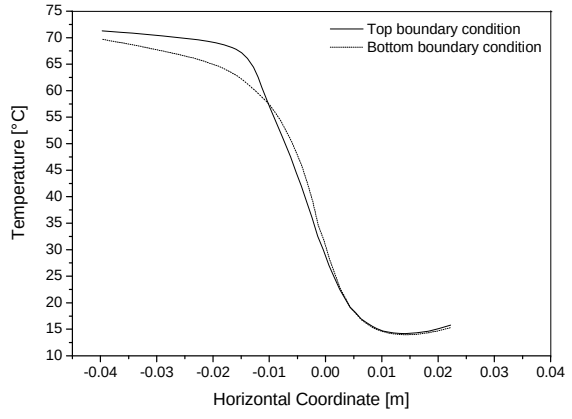

Figure 8: Boundary conditions for the "melting" case.

4. Numerical simulation: results and discussion

For simplicity, two dimensional conditions are assumed in the present numerical analysis since, according to [1,2], 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 glass tube due to the experimentally observed temperature variations outside this region were found to be negligible [1,2]. A central length of 80 mm has been considered for the simulations. Steady state conditions are only analyzed considering impermeable boundaries of the liquid-filled region and temperature profiles on the outer surface of the glass walls derived from the experiments in [2]. A non uniformly distributed regular mesh of 60x20 elements has been chosen for the computations of the three cases; see Figure 9.

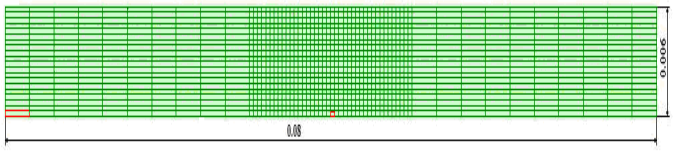

Figure 9: Finite element mesh used for the analysis of phase change in a Bridgman apparatus.

For the "no growth" case, the boundary conditions plotted in Figure 4 show that the horizontal distance between the locations of the phase change isotherm (58.09 °C) at the bottom and top of the glass tube is about 2.5 mm. Computed and experimental steady state solid-liquid interface positions are shown in Figure 10. 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 (± 0.5 mm). These numerical results are also quantitatively concordant to those reported in [1]. Moreover, Figure 11 shows the computed

steady state isotherms and streamlines obtained with FEM. The isotherms are deformed by the convection currents in the liquid phase. This isotherms distortion weakly propagates into the solid. The streamlines show the development of a main vortex. In general, the predicted velocity modulus is among the range of the experimental values derived from approximate observations of particle tracks. The numerical maximum velocity located at the mid-height of the glass tube in the vicinity of the phase change front was 1.22 mm/s, which reasonably agrees with the experimental measurement given in [2]. The steady state was reached at 480 s in the process time.

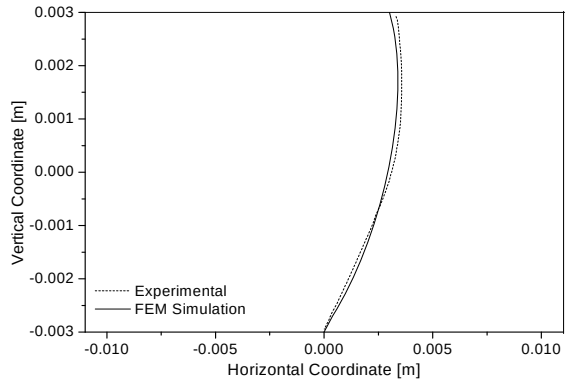

Figure 10: Steady state solid-liquid interface position for the "no growth" case.

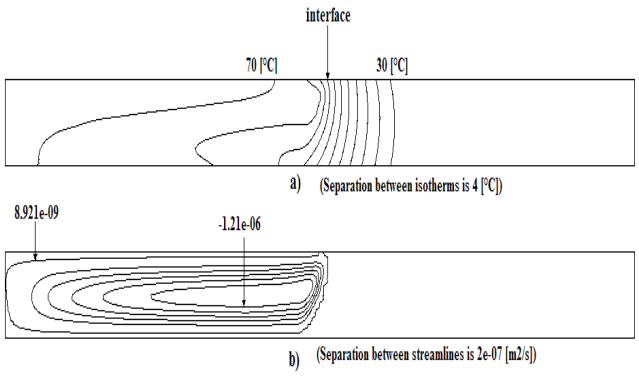

Figure 11: Steady state a) isotherms and b) streamlines computed with FEM for the "no growth" case.

For the "solidification" case, the boundary conditions plotted in Figure 6 show that the horizontal distance between the locations of the phase change isotherm (58.09 °C) at the bottom and top of the glass tube is about 5.5 mm. Computed and experimental steady state solid-liquid interface positions are plotted in Figure 12. Once again, the phase change front is influenced significantly by the convection which produces a great curvature due to the movement of the external jackets.

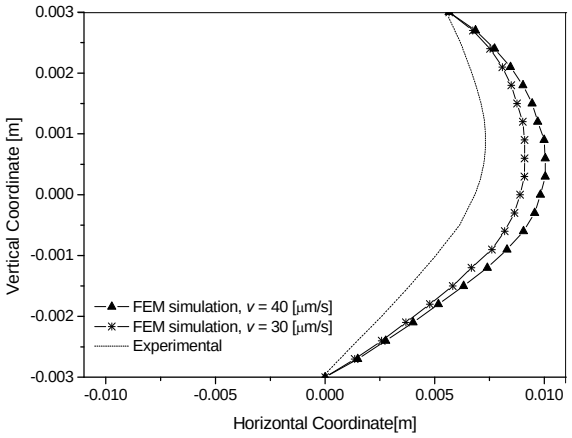

Figure 12: Steady state solid-liquid interface position for the "solidification" case.

In general, there is a good qualitative agreement between experimental and numerical phase change front which is more and less accurate at the glass walls and mid-height of the cavity, respectively. Furthermore, an additional simulation is performed considering a jacket's velocity of 30 μm/s in order to assess the influence of this variable on the phase change front position. As it can be seen, the fit of this curve with the experimental data improves a little. Moreover, Figure 13 shows the computed steady state isotherms and streamlines obtained with FEM. The isotherms are highly deformed by the convection currents due to the action of the external jackets. This distortion considerably propagates into the solid. The streamlines show the development of a main vortex. The numerical maximum velocity located at the mid-height of the glass tube in the vicinity of the phase change front is 0.89 mm/s. For

this case, the steady state was reached at 600 s in the process time.

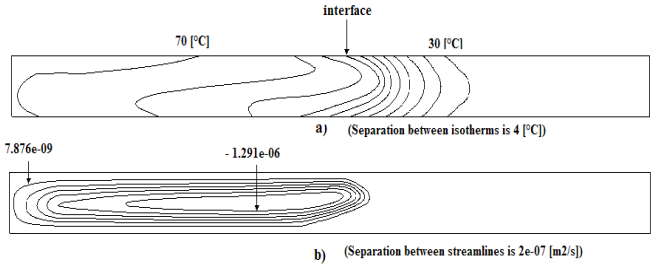

Figure 13: Steady state a) isotherms and b) streamlines computed with FEM for the "solidification" case.

For the "melting" case, the boundary conditions plotted in Figure 8 show that the horizontal distance between the locations of the phase change isotherm (58.09 °C) at the bottom and top of the glass tube is null. Computed and experimental steady state solid-liquid interface positions are plotted in Figure 14. As in the previous cases, the phase change front is influenced significantly by the convection which produces a great curvature due to the movement of the external jackets. In this case, the simulation is not able to capture the shape of the measured phase change front. Furthermore, a simulation is performed considering a jacket's velocity of -30 μm/s. As it can be seen, the fit of this curve with the experimental data improves a little. Moreover, Figure 15 shows the computed steady state isotherms and streamlines obtained with FEM. Once again, the isotherms are highly deformed by the convection currents due to the action of the external jackets. This distortion considerably propagates into the solid. The streamlines show the development of a main vortex. The numerical maximum velocity located at the mid-height of the glass tube in the vicinity of the phase change front is 1.20 mm/s. For this case, the steady state was reached at 500 s in the process time.

The results corresponding to these three cases are plotted together in Figure 16. It is clearly seen that, as already mentioned, the movement of the jackets ("solidification" and "melting" cases) produces a major curvature of the phase change front than that of a purely natural convection process ("no growth" case).

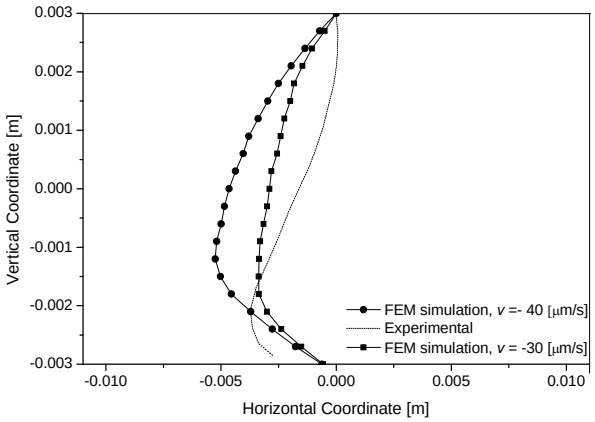

Figure 14: Steady state solid-liquid interface position for the "melting" case.

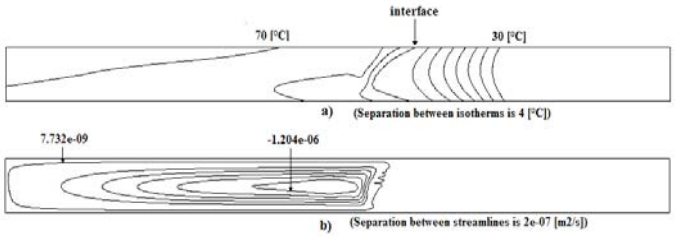

Figure 15: Steady state a) isotherms and b) streamlines computed with FEM for the "melting" case.

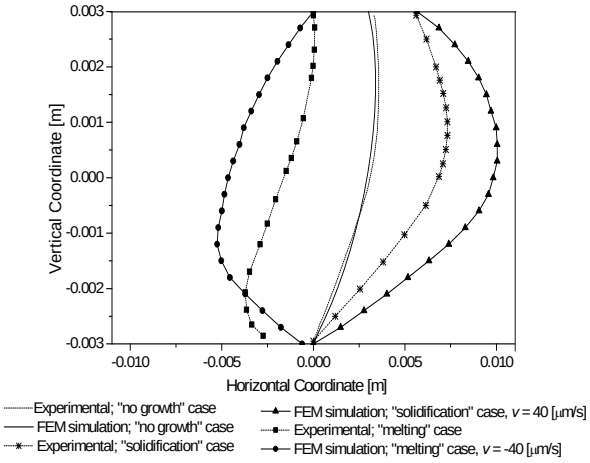

Figure 16: Steady state solid-liquid interface position for "no growth", "solidification" and "melting" cases.

5. Conclusions

The analysis of the succinonitrile phase change phenomenon that takes place in a horizontal Bridgman test has been presented using the finite element method as numerical approach. Three cases were particularly studied in which the numerical predictions were compared with the available experimental measurements. The simulation has provided very good predictions of the phase change front position for the "no growth" case. Some experimental-numerical discrepancies, however, were found for the "solidification" and "melting" cases. Further research must be carried out in order to find the reasons that could explain the differences between the experimental and numerical results for the "solidification" and "melting" cases.

Acknowledgements

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6. References

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