FRONT TRACKING TECHNIQUE ON A FIXED GRID IN MODELLING OF BINARY MIXTURE SOLIDIFICATION WITH NATURAL CONVECTION

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Summary. A novel front tracking method is presented in calculations of binary mixture solidification driven by conduction and natural convection. The method based on the local dendrite tip kinetics enables the detection of the under-cooled liquid zone in front of a curve joining the dendrite tips. Its results have been verified and validated through detailed comparisons with both: the predictions of the enthalpy-porous medium model and the PIV experimental findings.

Nowadays, it is commonly appreciated that natural convection plays a crucial role in formation of local micro- and macro-structures during solidification of binary systems. For over two decades various validate computer simulations of these two coupled and complex phenomena have become a fundamental tool for prediction of local flow patterns, temperature and concentration fields, supplementing or even replacing cumbersome time-consuming and expensive experimental findings.

The most popular macroscopic representation of transport phenomena in the two-phase region ('mushy zone') is based on the single domain approach (valid for liquid, solid and mushy zones), where this region is macroscopically represented by the enthalpy–porous medium model and underlying micro-structural evolution is incorporated via a map of solid fraction throughout the domain.

Yet, a novel front tracking technique on a fixed Cartesian grid, based on the kinetics of dendritic growth was developed recently [1,2,3,4]. Its results have been compared with the ones got from the enthalpy-porous medium model - in details for the case of solidification driven only by conduction [1,2,4] and preliminary when the thermal natural convection also occurs [3] - showing the superiority of the front tracking technique in the detection of the under-cooled zone and, thus, in potentially modelling of columnar/equiaxed grain structures [1,4].

The paper presents further development of this numerical technique in calculations of binary mixtures solidification driven by both conduction and natural convection as well as in the model verification and validation through its comparisons with both: the theoretical predictions by the enthalpy-porous medium approach and the experimental results got through the use of the PIV (Particle Image Velocimetry) technique [5].

A novel model of the advance of a columnar front and the growth of equiaxed grains, proposed in [1,3,4], is based on a front-tracking technique on a fixed grid and on the kinetics of dendrite growth. Mass-less marker particles are used to determine the interface evolution as a function of the local under-cooling. An initial position of each marker is assumed in accordance with both an initial state and thermal boundary conditions. A new position of each marker is then calculated from the time interval Δt and the growth velocity, which is a function of local under-cooling determined from a current temperature field. This dendrite kinetics relationship, which is fundamental in the model, can result from the theoretical considerations (e.g. [6]) or from experimental findings. A new interface position is then obtained by linear interpolation between each successive marker. So, it is assumed that the columnar front is a line joining dendrite tips. Next, the points at which this representation of the front intersects the grid-lines of the computational mesh are calculated. These points now become the new marker particles. Like in the classical single-domain approach, the single set of mass, momentum and energy conservation equations is used to get the velocity, pressure and temperature fields. But the commonly used total enthalpy concept is not applied here. Instead, the latent heat effect is considered by a careful definition of the source terms in the energy equation accounting for both: the advance of solidification front and subsequent thickening of the mushy zone within a control volume [1,3,4].

The fact that the kinetics of dendrite tips is exploited in the model, enables it to identify two regions between the equilibrium solidus and liquidus isotherms within a control volume that containing the interface, namely the columnar dendrite zone behind the dendrite tips and the under-cooled zone in front, where equiaxed structure can be formed. To show that the temporal shapes of all zones are given in Fig.1 for solidification of Al_2%wgt-Cu in a sand mould (interface heat transfer coefficient equal to $500 W/(m^2K)$) driven by pure conduction (the first three left columns) and also by thermal natural convection, showing the flow pattern (the remaining columns). Here the kinematics of dendrite tips is a theoretical parabolic function of the local under-cooling [6].

The verification and validation procedures for the front tracking model were further conducted through the detailed comparisons of its results with both: the enthalpy-porous medium model calculations and the experimental velocity field along with the front position identified from the PIV technique.

As an example problem the solidification, in a differentially heated square cavity, of 3.5%wgt NH_4Cl in water was simulated. The left vertical wall was kept at the initial temperature of $9.5^{O}C$ whereas the right one had a temperature of $-10^{O}C$. Figure 2 shows shapes and positions of the interface at four different times of the process, whereas the Figure 3 depicts the corresponding results from the enthalpy-porous medium model calculations.

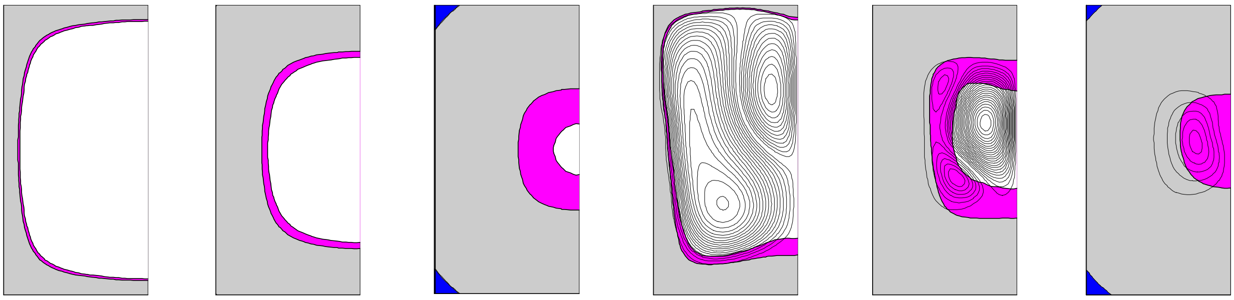

Fig.1. Solidification of Al_2%wgt_Cu in a sand mould: white – liquid phase, pink – under-cooled liquid zone, grey – mushy zone, dark blue- solid phase.

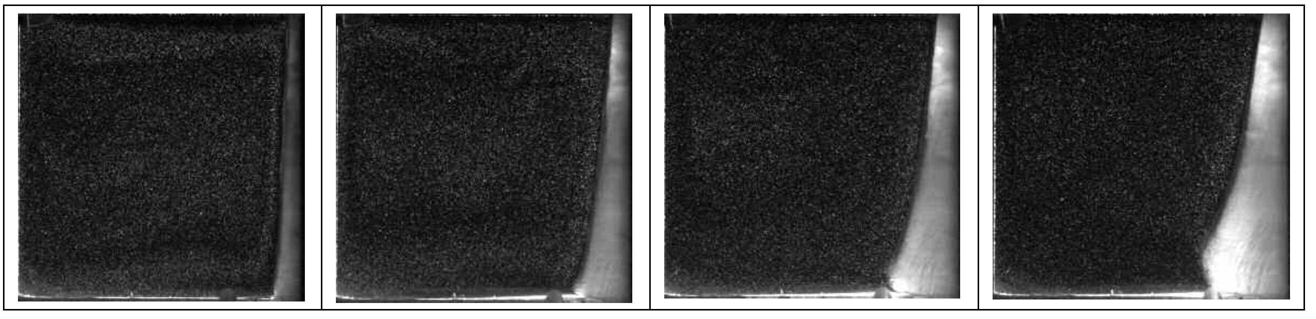

Fig.2. Experimental pictures: the seed and the temporal solid-liquid front position after 100s, 500s, 1000s and 2000s (from left to right) of solidification of 3.5%wgt aqueous solution of NH_4Cl.

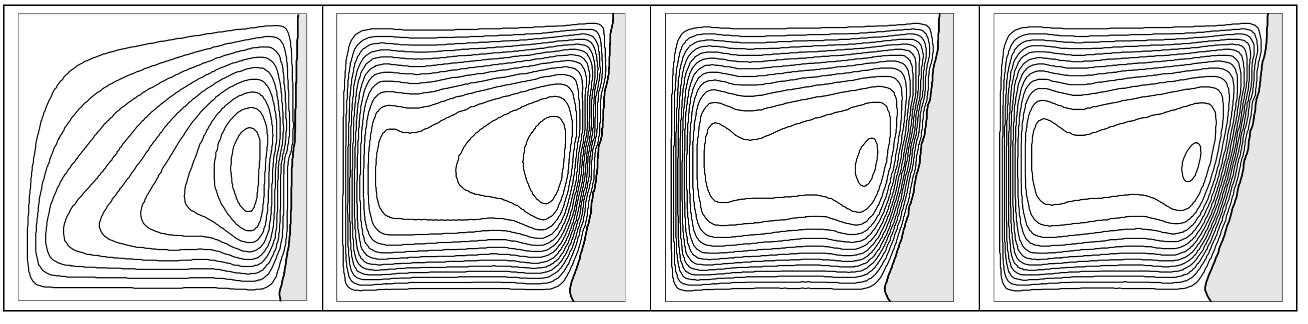

Fig.3 Enthalpy-porous medium model: the calculated flow pattern and solid phase shape after 100s, 500s, 1000s and 2000s (from left to right) of solidification of 3.5%wgt aqueous solution of NH_4Cl..

Kinematics of dendrite tips, used in the front tracking technique, has been obtained experimentally, i.e. from pictures of the temporal front shapes taken at short even time intervals using a high resolution camera. This allows specifying the local dendrite tips velocity as a function of time and position.

Detailed comparisons of the velocity field and front positions calculated by the front tracking technique with those presented above will be given in the paper. They will be followed by a short discussion concerning the physics of phenomena and the results of the validation procedure performed.

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