Int. J. Heat Mass Transfer. Vol. 36, No. 17, pp. 4095–4106, 1993
Printed in Great Britain

0017–9310/93 $6.00 + 0.00

Numerical simulation of convection/diffusion phase change problems—a review

A. A. SAMARSKII,† P. N. VABISHCHEVICH,† O. P. ILIEV‡ and A. G. CHURBANOV†

† Institute for Mathematical Modeling, Russian Academy of Sciences, Muisskaya Square 4, Moscow 125047, Russia

‡ Institute of Mathematics with Computer Center, Bulgarian Academy of Sciences, Acad. G. Bonchev str., bl. 8, Sofia 1113, Bulgaria

(*Received* 27 *May* 1993)

Abstract—A review of numerical techniques for the solution of heat and mass transfer problems with solid/liquid phase change is presented. The mathematical model for a description of a thermal field is based on the conventional Stefan approximation for the evaluation of phase change and the Navier–Stokes equations in the Boussinesq approximation for convective flows of a melt. Two basic approaches for the solution of these problems with a free boundary (phase change interface) are considered. The first approach is connected with interface-fitting algorithms (referred to in the work as variable grid methods), the second one with interface-smearing (fixed grid) methods. Fixed grid methods for the investigation of hydrodynamical phenomena in a varying calculation domain are constructed using various modifications of a penalty method.

1. INTRODUCTION

NOWADAYS many physical phenomena and technological processes can be investigated in detail due to the progress in computer performance and numerical methods. The number of publications devoted to the development of numerical methods for solving convection/diffusion phase change conjugate problems increases every year. In accordance with this fact the number of papers devoted to the numerical simulation of various physical and technological problems with heat and mass transfer including phase change increases too.

The earliest works on numerical simulation of phase change problems including convection are concerned with studying different metallurgical processes. Convection of a liquid metal becomes significant when the melting or solidification of relatively large metal volumes is considered [1, 2]. Now convection/diffusion phase change problems arise in mathematical modeling of metals and alloys casting or melting, crystal growth, plastic production, energy accumulation, geology, laser processing of metals, etc.

It is clear that a great deal of publications in this field need to be analyzed, comprehended and classified. Therefore, a number of surveys have been issued recently. In the work of Basu and Date [3] different formulations and classifications of melting or solidification problems with and without convection are discussed primarily from the physical viewpoint. Voller *et al.* [4] conducted an analysis of fixed grid numerical methods for prediction of melting/solidification phenomena without convection based on the English language literature only. Surveys of papers devoted to the mathematical modeling and experimental investigations of crystallization processes are published periodically by Viskanta (see for example [5]). Methodological aspects of the mathematical modeling of crystallization processes along with the quality and possibilities of software existing in this field are discussed in the survey by Kanan *et al.* [6].

The main purpose of the present paper is to discuss the state-of-the-art in modeling convection/diffusion phase change using the up-to-date level of applied and computational mathematics. Most of the works published in this field will be analyzed, including papers in Russian which are practically unknown for readers in English. A number of applications is also provided.

Investigating convection/diffusion processes during melting or solidification, the following assumptions are adopted in the present paper:

- convenient parabolic heat transfer equation based on the Fourier law is used;
- Stefan's conditions take place on the phase change boundary for pure substance solidification and various models of a mushy region are employed for alloys and mixtures solidification;
- thermal and/or solutal convection in the liquid phase are governed by the Navier–Stokes equations in the Boussinesq approximation for laminar flows;
- the density variation due to the phase change is neglected;
- a flow in a mushy region is modeled using the simplest models—say, in the Darcy–Boussinesq approximation for porous media.

It should be noted that the above mentioned convection/diffusion phase change problems are essen-

NOMENCLATURE

C	specific heat at constant pressure
h	enthalpy
k	thermal conductivity
K	permeability of a porous medium
L	phase change enthalpy
P	pressure
S	source term in transport equations
t	time
T	temperature
T^*	phase change temperature
$\mathbf{v} = (u, v, w)$	velocity vector
(x, y, z)	Cartesian coordinates.

Greek symbols

Δ	Laplace operator
ε	extension parameter in the fictitious regions method
μ, μ', ν	dynamic, volumetric and kinematic viscosities
ρ	density
σ	velocity–strain tensor
Ψ	solid phase volume fraction
ψ	stream function
ω	vorticity.

Subscripts

ef	effective value
s, l	solid and liquid phases, respectively
n	normal component.

tially nonlinear ones. First, they are nonlinear due to convective terms in the momentum and energy equations. Secondly, thermophysical properties of considered substances often depend on the temperature. And finally, nonlinearity in the problems under consideration is caused by the existence of a free boundary—a phase change interface. The location of the boundary is a priori unknown and depends on the solution of the considered problem. The first two kinds of nonlinearity are well known and widely discussed in the literature on numerical methods for computational fluid dynamics and thermophysics. A host of papers and monographs is devoted to these nonlinearities of common knowledge (e.g. [7–11]) and so these points will be omitted here.

The present paper is organized as follows. The basic equations governing the heat and mass transfer and phase change are presented in the second part. In the third part a short review is given on existing numerical methods for solving the pure heat conduction equation, describing melting or solidification problems without convection. Numerical methods based on the interface-fitting technique are discussed in the fourth part along with their applications to convection/diffusion phase change problems of practical interest. The fifth part covers the fixed grid numerical methods for solving convection/diffusion phase change problems as well as their application to several physical and technological processes. The last part is devoted to some conclusions.

2. GOVERNING EQUATIONS

The equations under the consideration governing the heat and mass transfer processes during the liquidus–solidus and solidus–liquidus phase change are based on the conservation laws for the energy, mass and momentum [12]. Hereinafter in the work we shall write 'solidification' meaning that melting is governed by the same equations as solidification. Concerning the solidification processes we shall consider the Stefan problem for pure substances, that is, the phase change occurs at fixed temperature $T = T^*$ and there is a smooth phase change boundary $\Gamma(t)$ in this case. On the other hand, considering alloys and mixtures which solidify in a temperature interval, we shall take into account the existence of a spatial mushy (solid and liquid) region between solid and liquid phases.

2.1. *Energy equation*

The temperature field in the solid phase is governed by usual heat equation:

$$\rho C_s \frac{\partial T_s}{\partial t} = \operatorname{div}(k_s \operatorname{grad} T_s) + S_s^f. \tag{1}$$

In general form the convection/diffusion heat transfer equation for the liquid and mushy (if it exists) regions can be written as follows:

$$\rho C_l \left(\frac{\partial T_l}{\partial t} + (\mathbf{v}, \operatorname{grad}) T_l \right) = \operatorname{div}(k_l \operatorname{grad} T_l) + S_l^f. \tag{2}$$

For pure substances the temperature on a smooth phase change interface $\Gamma(t)$ is fixed and equal to a constant temperature of phase change:

$$\Gamma(t) = \{(x, y, z) | T(x, y, z, t) = T^*\}. \tag{3}$$

This relation can be used to determine this boundary. Standard Stefan boundary conditions (continuity of the temperature and jumping of the heat flux) are satisfied on this boundary:

$$[T] = 0, \quad (x, y, z) \in \Gamma(t), \tag{4}$$

$$\left[k \frac{\partial T}{\partial n} \right] = -\rho L V_n, \quad (x, y, z) \in \Gamma(t). \tag{5}$$

Here $[\phi]$ stands for the jump of the quantity ϕ through

$\Gamma(t)$ from the solid phase to the liquid one. Note that conditions (4) and (5) can be implemented in the heat conduction equation via a suitable source term. In this case instead of equations (1)–(5) one can consider a single equation, governing the convection/diffusion heat transfer in the whole considered domain—solid, mushy and liquid regions:

$$\rho C\left(\frac{\partial T}{\partial t}+(\mathbf{v}, \operatorname{grad}) T\right)=\operatorname{div}(k \operatorname{grad} T)+S^{*}. \tag{6}$$

Clearly the velocity $\mathbf{v}$ is identically equal to zero $\mathbf{v} \equiv 0$ in the solid phase. Equation (6) can be used for calculating solidification of pure substances as well as alloys by means of appropriate source term S^{*}. Let us consider these possibilities in more detail.

First, usage of the effective heat capacity will be demonstrated. Conditions (4) and (5) can be automatically satisfied for the following source term $S^{*}=S^{T}-\rho L \delta(T-T^{*})(\partial T/\partial t)$, as it is shown in refs. [13–15] for the Stefan problem (that is, for pure substances solidification). Here S^{T} denotes sources which are not connected with the latent heat release during the phase change. Secondly, for the alloys solidification the source term can be written as $S^{*}=S^{T}-\rho L(\mathrm{d}\Psi/\mathrm{d}T)$ (see, for instance, [1]). Now equation (6) can be rewritten as follows:

$$\rho C_{\mathrm{ef}}\left(\frac{\partial T}{\partial t}+(\mathbf{v}, \operatorname{grad}) T\right)=\operatorname{div}(k \operatorname{grad} T)+S^{T}, \tag{7}$$

where

$$C_{\mathrm{ef}}=\begin{cases} C+L\delta(T-T^{*}) & \text{for pure substances,} \\ C+L\dfrac{\mathrm{d}\Psi}{\mathrm{d}T} & \text{for alloys.} \end{cases} \tag{8}$$

Numerical solution of PDEs with a coefficient including the Dirac function needs the development of special numerical techniques. Therefore, the enthalpy function h can be introduced and instead of equation (7) we can consider

$$\rho\left(\frac{\partial h}{\partial t}+(\mathbf{v}, \operatorname{grad}) h\right)=\operatorname{div}(k \operatorname{grad} T)+S^{T} \tag{9}$$

where

$$h=\int_{0}^{T} C_{\mathrm{s}}\,\mathrm{d}T, \quad T \leqslant T^{*}, \tag{10}$$

$$h=h(T^{*})+L+\int_{T^{*}}^{T} C_{\mathrm{l}}\,\mathrm{d}T+L, \quad T>T^{*}. \tag{11}$$

Merits and demerits of numerical techniques, based on equations (7) and (9) are discussed in many papers (basically for the pure heat conduction). In particular, various approaches for smearing the enthalpy discontinuity in equations (7) and (9) and their influence on the solution accuracy are examined in ref. [16]. In the present paper we shall not discuss this topic, referring readers to the extensive review [4] for more details.

2.2. *Momentum and continuity equation*

Now consider the models describing convective motion of a melt. The Navier–Stokes equations for a laminar incompressible viscous flow can be written as:

$$\frac{\partial \rho \mathbf{v}}{\partial t}+\operatorname{div}(\rho \mathbf{v}\mathbf{v})=2\operatorname{div}(\mu \sigma)-\operatorname{grad} P - \operatorname{grad}\left(\left(\tfrac{2}{3}\mu-\mu'\right)\operatorname{div}\mathbf{v}\right)+S^{V} \tag{12}$$

$$\frac{\partial \rho}{\partial t}+\operatorname{div}(\rho \mathbf{v})=0. \tag{13}$$

The Boussinesq approximation is in common use to describe convective motion of a melt. In this case we have:

$$\frac{\partial \mathbf{v}}{\partial t}+(\mathbf{v}, \operatorname{grad})\mathbf{v}=-\frac{1}{\rho}\operatorname{grad} P+\operatorname{div}(\nu \operatorname{grad}\mathbf{v})+S^{\mathrm{v}} \tag{14}$$

$$\operatorname{div}\mathbf{v}=0. \tag{15}$$

Stream function–vorticity variables (ψ, ω) are usually preferred in computational fluid dynamics for solving 2D problems—see, for example, [7–11]. Thus, instead of equations (14) and (15) in primitive variables (velocity–pressure), the following equations in the (ψ, ω)-formulation can be used:

$$\frac{\partial \omega}{\partial t}+(\mathbf{v}, \operatorname{grad})\omega=\operatorname{div}(\nu \operatorname{grad}\omega)+S^{\omega} \tag{16}$$

$$\Delta\psi=-\omega \tag{17}$$

where $\Omega=\operatorname{rot}\mathbf{v}$, $\Omega=(0, 0, \omega)$, $\mathbf{v}=\operatorname{rot}\Psi$, $\Psi=(0, 0, \psi)$. In some instances one can employ the fourth-order stream function equation:

$$\frac{\partial \Delta\psi}{\partial t}+(\mathbf{v}, \operatorname{grad})\Delta\psi=\operatorname{div}(\nu \operatorname{grad}\Delta\psi)+S^{\psi}. \tag{18}$$

Note, that the computational aspects of the usage of various Navier–Stokes equations formulations are widely analyzed in the literature (e.g. [7–11, 17, 18]) and therefore they will not be discussed here. It is more important for us to highlight existing models of melt motion for a mushy region. The simplest model is based on the so-called porous medium approach. In this case a mushy region is considered as a porous medium and the Darcy–Boussinesq equations are utilized to describe here a melt flow. Note, that in such models the emphasis is on the determination of a relationship between permeability and species volume fraction.

For convenience of presentation we shall discuss different numerical techniques for prediction of convection/diffusion phase change on the test problem of metal (or alloy) solidification in a rectangular cavity cooled from the right side, whereas the top and bot-

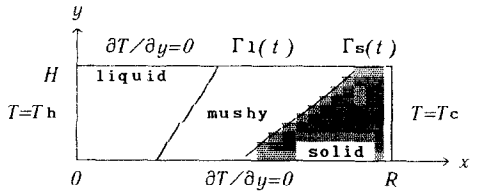

FIG. 1.

tom are thermally insulated (see Fig. 1). It is clear, that only a smooth boundary exists between solid and liquid phases when one considers the pure substance solidification. Moreover, if one considers the classical Stefan problem (without convection) with the above mentioned boundary conditions, the phase change interface will be plain and parallel to the axis $0y$. So, a distinction between computed phase change interface for the convection/diffusion problem and the plain interface for the classical Stefan problem will demonstrate the impact of melt convection on heat transfer.

3. SOLUTION OF HEAT CONDUCTION EQUATION WITH PHASE CHANGE

Now we briefly discuss numerical methods for the solution of the phase change problems when convection is negligible and can be ignored.

The Stefan problem has been investigated by many authors—see, for instance, monographs [15, 19–22]. This problem can only be solved analytically in the simplest cases (e.g. [13, 23]) and so in most cases it has to be calculated numerically. Numerical methods for solving such problems with free (unknown) boundary [24] can be generally divided into two groups. The first group consists of algorithms with explicit capturing of the unknown phase change interface (such methods sometimes are called 'variable grid (or domain) methods'). The second group includes the methods without interface fitting which are based on smearing a free boundary in some fashion (following [3, 4] we will call them 'fixed grid numerical methods').

3.1. *Variable grid methods*

As was mentioned above, in the numerical methods from this group the exact location of the phase change interface is evaluated on a grid at every time-level. In these methods a phase change interface is captured in some grid point (dynamical, interface-fitting grids are employed). Therefore, it is necessary to utilize grids with a non-uniform spacing in the methods of this group.

Solving 1D problems one can choose another approach. To capture phase change interface in this case, we can use a uniform spatial grid, but a non-uniform time-step. Such an approach (fitting a phase change boundary in a node of a spatial grid using a variable time-step) is suggested in refs. [25, 26]. Let us note, that this approach has been repeatedly employed to solve two-phases and multi-phases 1D problems, but it is not applicable for the solution of multidimensional problems.

The most widespread variable methods are based on the dynamical grids, where some fixed grid nodes move with the phase change boundary during a time evolution and other nodes are dynamically reconstructed at every time-level. Such an approach is suggested in refs. [27, 28]. From the new works in this field we shall point out the work [29], where this approach is applied for 2D problems using a modern technique for grid adaptation.

A special feature of the Stefan and Stefan-like problems are non-uniform conditions (3)–(5), relating two phases. A numerical method, based on the simple layer potential theory is developed in refs. [30, 31] to implement these conditions more precisely. More details of this class of methods are presented in monograph [32].

3.2. *Fixed grid methods*

Usage of variable grid numerical methods to solve multidimensional phase change problems is algorithmically complicated and leads to large computational cost, so fixed grid numerical methods are in common use for solving such problems. Beginning with the works of Samarskii and Moiseenko [33] and Budak *et al.* [34] for the temperature formulation (7) and with the work [35] for the enthalpy formulation (9) a number of fixed grid numerical methods have been developed and applied for studying pure conduction phase change problems. The essence of the method suggested in ref. [33] for the solution of the Stefan problem is the introduction of the effective heat capacity. Instead of

$$\rho(C+L\delta(T-T^*))\frac{\partial T}{\partial t}=\operatorname{div}(k\operatorname{grad}T) \tag{19}$$

the next equation is to be solved

$$\rho\tilde{C}\frac{\partial T}{\partial t}=\operatorname{div}(k\operatorname{grad}T). \tag{20}$$

Effective heat capacity $\tilde{C}$ is chosen from the condition of energy conservation over some temperature interval, including temperature of phase change:

$$\int_{T^*-\eta}^{T^*+\eta}(C+L\delta(T-T^*))\,\mathrm{d}T=\int_{T^*-\eta}^{T^*+\eta}\tilde{C}(T)\,\mathrm{d}T. \tag{21}$$

For example, one can set

$$\tilde{C}=C+\frac{L}{2\eta}. \tag{22}$$

More details of choosing the value of η in the above equation are discussed in ref. [33] along with some different approximations for $\tilde{C}$. Note, that some variants of the enthalpy formulation for the Stefan problem are practically identical to the method [33]—see,

for example, review [3, p. 182]. At the end of this paragraph it is useful to point out that one can find a comprehensive review of publications in English connected with this topic in the above mentioned work [4].

4. PREDICTION OF CONVECTION/DIFFUSION PHASE CHANGE. VARIABLE GRID METHODS

For convenience we shall divide methods of this group into some subgroup. To the first subgroup we shall refer the methods which are based on a transformation of the considered irregular physical domain onto a rectangular one introducing new independent variables. The second subgroup includes the methods based on unstructured or deforming grids in the initial physical domain. Finally, to the last subgroup we shall refer local adaptation methods. It is clear that there are many common features between all these groups and a particular numerical algorithm can be considered variously.

4.1. *Domain transformation techniques*

Nowadays a great deal of numerical algorithms for the solution of 2D convection/diffusion phase change problems with moving free boundary use a transformation of the domain, occupied by a melt (i.e. liquid phase). Doing so, new independent variables have to be introduced. An example is conformal mapping of the initial irregular domain. It is necessary to point out that we must consider transient (time-dependent) calculation domain transformation (at every time-level of computations) since the domain occupied by a melt is evolving in time. Various numerical techniques, say, FDM or FEM, can be employed for solving transformed equations.

Let us demonstrate this approach applying it to our test problem and using stream function–vorticity formulation of the Navier–Stokes equations (16) and (17) in Cartesian coordinates. In this case the domain $G^*(t)$ occupied by a liquid phase at the moment t can be transformed into a regular domain Ω via introducing new variables $\xi = \xi(x, y, t)$ and $\eta = \eta(x, y, t)$. Following the above mentioned assumptions the transformed vorticity equation can be written as

$$\frac{\partial \omega}{\partial t} + \frac{1}{J}\left(\frac{\partial x}{\partial \eta}\frac{\partial y}{\partial t} - \frac{\partial y}{\partial \eta}\frac{\partial x}{\partial t}\right)\frac{\partial \omega}{\partial \xi} + \frac{1}{J}\left(\frac{\partial y}{\partial \xi}\frac{\partial x}{\partial t} - \frac{\partial x}{\partial \xi}\frac{\partial y}{\partial t}\right)\frac{\partial \omega}{\partial \eta} + \frac{1}{J}\frac{\partial (U\omega)}{\partial \xi} + \frac{1}{J}\frac{\partial (V\omega)}{\partial \eta} = \frac{1}{J}\frac{\partial}{\partial \xi}\left(\frac{Pr}{J}\left(\alpha\frac{\partial \omega}{\partial \xi} - \beta\frac{\partial \omega}{\partial \eta}\right)\right) + \frac{1}{J}\frac{\partial}{\partial \eta}\left(\frac{Pr}{J}\left(\gamma\frac{\partial \omega}{\partial \eta} - \beta\frac{\partial \omega}{\partial \xi}\right)\right) + Ra \cdot Pr \cdot S^{\omega}(\xi, \eta). \tag{23}$$

Metric coefficients α, β, γ, velocity components u, v and Jacobian J are defined as

$$\alpha = \left(\frac{\partial x}{\partial \eta}\right)^2 + \left(\frac{\partial y}{\partial \eta}\right)^2, \tag{24}$$

$$\beta = \frac{\partial x}{\partial \xi}\frac{\partial x}{\partial \eta} + \frac{\partial y}{\partial \xi}\frac{\partial y}{\partial \eta}, \tag{25}$$

$$\gamma = \left(\frac{\partial x}{\partial \xi}\right)^2 + \left(\frac{\partial y}{\partial \xi}\right)^2, \tag{26}$$

$$u = \frac{\partial \psi}{\partial \eta}, \quad v = -\frac{\partial \psi}{\partial \xi}, \tag{27}$$

$$J = \frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \eta} - \frac{\partial x}{\partial \eta}\frac{\partial y}{\partial \xi}. \tag{28}$$

Other transformed equations can be derived in a similar way.

Particular emphasis must be placed on the fact that in the general case construction of mapping $\xi = \xi(x, y, t)$ and $\eta = \eta(x, y, t)$ is a very important and complicated problem itself. This transformation can be defined explicitly only for the simplest cases. Say, it can be simple stretching lengthwise of one of the spatial coordinates. From the viewpoint of grid generation (see, for instance [8, 9, 36, 37]) this simple approach corresponds to algebraical methods for grid generation. In general cases it is necessary to solve a couple system of PDEs at every time-level for grid constructing [36–38]. This procedure can require more computational cost than solving the transport equations themselves. That is why some additional assumptions are utilized to simplify determination of transformation $\xi = \xi(x, y, t)$ and $\eta = \eta(x, y, t)$.

Concerning convection/diffusion phase change problems general type transformations $\xi = \xi(x, y, t)$ and $\eta = \eta(x, y, t)$ have been used in refs. [39, 40]. This approach is also employed in ref. [41] for the numerical study of solidification of a water filled porous medium.

Let us return now to the above mentioned test problem (see Fig. 1). In this particular case the domain occupied by a liquid phase is a curvilinear quadrangle with three fixed and one free boundaries. It allows us to use the simplest non-uniform stretching of the domain $G^*(t)$ lengthwise of the direction x with a stretching coefficient depending on the coordinate y. The resulting calculation domain in this case is the rectangle Ω, $\Omega = \{(\xi, \eta): 0 \leqslant \xi \leqslant 1, 0 \leqslant \eta \leqslant H\}$. Taking into account that $(\partial y/\partial \xi) = 0$ and $\xi = \xi(x, y, t)$, $\eta = \eta(x, y, t)$ are defined explicitly there is no problem to transform equation (23) and other equations for this test problem.

Amongst the first papers where this simplified algorithm has been used for the solution of the test problem are refs. [42, 43]. The so-called quasi-stationary approach was employed in these works: it was assumed that the phase change interface was frozen between two discrete time moments t and $t+\Delta t$ and

so it is evaluated from the Stefan condition only at these discrete moments. A FDM approach has been used there to discretize the equations. The numerical algorithm was based on an alternating direction implicit (ADI) method for parabolic equations and a successive overrelaxation (SOR) method for the discrete elliptic stream function equation. It should be noted that the 'stretching' approach can be implemented using any other suitable finite-difference numerical methods for solving problems of mathematical physics (e.g. [44–47]). Viskanta and coworkers have utilized this approach for prediction of solidification and melting of a number of various concrete materials. Fine agreement with measured data have been obtained in these numerical experiments [48, 49].

A similar approach is applied in ref. [50] to solve heat and mass transfer equations in a single phase (liquid) and two-phase (liquid + vapor) regions for a test problem involving boiling and natural convection in a porous medium. We shall highlight some other works applying this approach to the problems of practical interest. The ice melting process in a porous cavity heated from below is investigated numerically in ref. [51]. Numerical analysis is presented in ref. [52] for horizontal solidification of binary alloys in a rectangular enclosure involving mutual diffusion of species (thermal and solutal convection are considered). Pure metal melting near a hot vertical wall is studied in ref. [53]. Influence of buoyancy-driven and thermocapillary (Marangoni) convection on pure metal solidification is discussed in ref. [54]. A parametric investigation of thermal and hydrodynamic fields is presented in ref. [55] for zonal melting of $NaNO_3$. Numerical study of pure substance melting involving convection has been conducted in ref. [56], whereas analysis of influence of thermal and Marangoni convection on pure metal solidification has been done in ref. [57].

As noted above, the quasi-stationary approach has been used in cited papers – a phase change interface is frozen at time between t and $t+\Delta t$ and its new location at the time moment $t+\Delta t$ is evaluated from the Stefan conditions (4), (5) and the updated temperature field after the determination of all other variables. It is clear that there is some time-step restriction in this approach with phase change interface freezing due to its explicit property. A more efficient approach is developed in ref. [58], where the location of phase change interface is calculated simultaneously with all other governing equations in an implicit fashion. A much higher time-step can be used in this case.

4.2. *Unstructured deforming grids*

Contrary to the previous group with explicit capturing of a phase change interface we now consider numerical methods which are based on the solution of the initial (non-transformed) equations using unstructured deforming grids. Note that distinctions between the previous and currently considered subgroups often exist only during the discretization of differential equations and the same difference equations can be obtained in both cases.

A new approach with an unstructured interface-fitting grid to be designed at every time-level is described in ref. [59]. A control volume method is used to obtain an implicit difference scheme. It should be noted that the cells adjacent to the interface in a liquid phase are triangular whereas all others are rectangular. Calculations at every time-level are performed as follows: first, a new phase change interface location is evaluated from the Stefan conditions (quasi-stationary approach), secondly, a new grid is generated, thirdly, the values of variables are interpolated on the new grid and so on. Development of the above mentioned method is continued in ref. [60]. Note that deforming finite elements can also be used for discretization of PDEs. Such an approach is employed in ref. [61].

4.3. *Local adaptation methods*

Here we shall briefly discuss the works where a phase change interface is determined explicitly and governing equations are accurately approximated near to the interface points of a fixed grid. For example, such an algorithm is proposed in ref. [62], where laser melting processes are considered. A bit simpler and therefore less accurate technique, based on the SIMPLE procedure, is described in refs. [63, 64]. One of the basic assumptions used in these works is that velocity components have small values in the vicinity of an interface and therefore convection can be neglected there. A similar algorithm has been used in refs. [65–67]. In fact the essence of this approach is that a smooth phase change interface is approximated by a polygonal line through the grid points.

Numerical methods with composite grids can be also considered in the framework of this subgroup (see, for instance, [68]). The essence of the composite grid technique is to construct a local moving orthogonal interface-fitting grid in addition to the basic grid for a whole computation domain. Some features of the computational implementation of this technique are discussed in ref. [69].

5. CONVECTION/DIFFUSION PHASE CHANGE PREDICTION. FIXED GRID METHODS

As already noted, in most papers on numerical simulation of convection/diffusion phase change it is assumed that a melt can be considered as an incompressible viscous fluid and a flow is a laminar one. In addition, it is assumed that the density has no changes due to phase change and therefore the simplest boundary condition for the velocity can be used on a phase change interface [70]. Considered in this paragraph are numerical methods which we shall divide into large subgroups depending on the mathematical models used to describe a melt flow in a liquid phase. The so-called primitive variables (velocity–pressure) are

used in the methods belonging to the first subgroup. To the second subgroup we shall assign numerical methods based on the stream function–vorticity formulation.

Let us note, that different scientists (mainly mathematicians and engineers) consider the mathematical modeling of convection/diffusion phase change problems from various points of view and use distinct terminology and result interpretation for the same situation. In this paper we shall consider fixed grid numerical methods only from the mathematical viewpoint, although some pure physical reasons can be used to describe a solid phase. In our opinion a convenient classification of the fixed grid numerical methods can be done using a general approach for solving mathematical physics problems in irregular domains which is known as the fictitious regions method (FRM). The fictitious regions method was suggested by Saul'yev in 1960 for solving elliptical problems [71]. The essence of this method is described in the monograph [72], and a general review of applications is presented in ref. [73]. The mostly complete description of the fictitious regions method and its applications to hydrodynamics problems can be found in the monograph [74].

5.1. *Primitive variables*

We start with the primitive variables formulation (u, v, P) for solving convection/diffusion phase change problems on fixed grids. Two variants of the FRM can be constructed in this case: the first of them is based on the continuation of the coefficient at lower-order derivatives and the second approach uses the continuation of the coefficient at the highest-order derivatives. Only the first variant has yet been published in connection with numerical simulation of the convection/diffusion phase change processes.

Let us briefly explain the first variant. Instead of (14), (15) for the irregular time-dependent domain $G^*(t)$ we consider for the whole rectangular computation domain G the following equations:

$$\frac{\partial \mathbf{v}_\varepsilon}{\partial t} + (\mathbf{v}_\varepsilon, \operatorname{grad})\,\mathbf{v}_\varepsilon = \frac{1}{\rho}\operatorname{grad} P_\varepsilon + \operatorname{div}(\nu \operatorname{grad} \mathbf{v}_\varepsilon) - C_\varepsilon \mathbf{v}_\varepsilon + S_\varepsilon^{\mathbf{v}} \quad (29)$$

$$\operatorname{div} \mathbf{v}_\varepsilon = 0. \quad (30)$$

Here the continuation coefficient C_ε and the right hand side $S_\varepsilon^{\mathbf{v}}$ are chosen like this:

$$C_\varepsilon = \begin{cases} 0, & (x, y) \in G^*(t), \\ \varepsilon^{-2}, & (x, y) \in G/G^*(t). \end{cases} \quad (31)$$

$$S_\varepsilon^{\mathbf{v}} = \begin{cases} S^{\mathbf{v}}, & (x, y) \in G^*(t), \\ 0, & (x, y) \in G/G^*(t) \end{cases} \quad (32)$$

where ε is sufficiently small. It is clear that C_ε and $S_\varepsilon^{\mathbf{v}}$ can be formulated in various ways for particular problems.

It should be noted that the fictitious regions method of the form (29)–(32) is well known and has been used for many years. A mathematical validation of the method is provided in ref. [75]. More precisely, there is obtained the following accuracy estimate for the approximate $\mathbf{v}_\varepsilon$ and the correct $\mathbf{v}$ solutions in this work for steady-state and unsteady incompressible viscous fluid flow problems:

$$\|\mathbf{v}_\varepsilon - \mathbf{v}\| \leqslant \text{const.}\, \varepsilon^{1/2} \quad (33)$$

in corresponding norms.

In more recent publications this approach is called the 'porous medium model'. Really, the term $C_\varepsilon \mathbf{v}_\varepsilon$ in equation (29) can be interpreted as the resistance force for fluid motion in a porous medium. It is well known that eliminating inertia terms we obtain the Darcy–Boussinesq equation for a porous medium in the following form:

$$\mathbf{v} = -\frac{K}{\mu}\operatorname{grad} P. \quad (34)$$

Combining equations (34) and (14) and continuing the coefficient K by zero value in a liquid phase and a very high value in a solid phase, we can obtain a single equation similar to (29), which describes considered processes in the whole domain including liquid and solid phases. A similar approach can be applied for a two-phase zone too.

More details of the 'porous medium model' are presented in refs. [76–78], where the enthalpy formulation is employed for the energy equation and pure substance solidification in a cavity is considered. The same approach has been used in ref. [79] for the investigation of alloy solidification, where the mushy region is considered as a porous medium. This approach was used by the same authors and their colleagues for studying some particular processes. Thus, a laminar unsteady pure substance flow through cooled tubes is investigated numerically in ref. [80] involving solidification on the tube walls. Pure gallium melting in a cavity with a heated side wall is calculated in ref. [81] and compared with measurements. Pure tin solidification is investigated in ref. [82]. Thermosolutal convection in a liquid phase is considered in ref. [83].

It is apparent that the 'porous medium' model is widely used for the numerical simulation of various convection/diffusion phase change processes. At the same time a number of works are devoted to the improvement of the numerical algorithm. The emphasis is on the evaluation of the permeability K (equation (34)) in a porous medium and its continuation in a solid phase. Numerical results from [84] indicate that the predicted thermal field during convection/diffusion phase change essentially depends on the evaluation of the effective permeability K and a new technique for choosing K is suggested in this work. Further, more correct determination of the permeability is developed in ref. [85], where the nature of the mushy region is taken into account. It is necessary

to note the last works of the same authors in this field [86, 87]. It should be noted that the technique suggested in ref. [84] is based on the previous works performed by Bennon and Incropera.

Another direction in the developing numerical techniques for the prediction of convection/diffusion phase change is the use of more accurate methods. Shyy and Chen [88] presented an algorithm based on nonorthogonal coordinates and adaptive grids. Solidification in a cavity heated from one side has been considered using the 'porous medium' model. It is interesting that Cartesian and curvilinear velocity components are used simultaneously in this method. Dimensionless equations in this case can be written in general form as:

$$\frac{\partial U}{\partial \xi} + \frac{\partial V}{\partial \eta} = 0, \tag{35}$$

$$\frac{1}{J}\frac{\partial (Uu)}{\partial \xi} + \frac{1}{J}\frac{\partial (Vu)}{\partial \eta} = \frac{Pr}{J}\left(\frac{\partial}{\partial \xi}\left(\frac{1}{J}\left(q_1\frac{\partial u}{\partial \xi} - q_2\frac{\partial u}{\partial \eta}\right)\right) + \frac{\partial}{\partial \eta}\left(\frac{1}{J}\left(-q_2\frac{\partial u}{\partial \xi} + q_3\frac{\partial \mu}{\partial \eta}\right)\right)\right) - \frac{1}{J}\left(y_\eta\frac{\partial p}{\partial \xi} - y_\xi\frac{\partial p}{\partial \eta}\right) + Au, \tag{36}$$

$$\frac{1}{J}\frac{\partial (Uv)}{\partial \xi} + \frac{1}{J}\frac{\partial (Vv)}{\partial \eta} = \frac{Pr}{J}\left(\frac{\partial}{\partial \xi}\left(\frac{1}{J}\left(q_1\frac{\partial v}{\partial \xi} - q_2\frac{\partial v}{\partial \eta}\right)\right) + \frac{\partial}{\partial \eta}\left(\frac{1}{J}\left(-q_2\frac{\partial v}{\partial \xi} + q_3\frac{\partial v}{\partial \eta}\right)\right)\right) - \frac{1}{J}\left(x_\xi\frac{\partial p}{\partial \eta} - x_\eta\frac{\partial p}{\partial \xi}\right) + Av + Ra\cdot Pr\cdot \phi, \tag{37}$$

$$\frac{1}{J}\frac{\partial (U\phi)}{\partial \xi} + \frac{1}{J}\frac{\partial (V\phi)}{\partial \eta} = \frac{1}{J}\left(\frac{\partial}{\partial \xi}\left(\frac{1}{J}\left(q_1\frac{\partial \phi}{\partial \xi} - q_2\frac{\partial \phi}{\partial \eta}\right)\right) + \frac{\partial}{\partial \eta}\left(\frac{1}{J}\left(-q_2\frac{\partial \phi}{\partial \xi} + q_3\frac{\partial \phi}{\partial \eta}\right)\right)\right) - \frac{1}{J\cdot St}\left(\frac{\partial}{\partial \xi}(U\cdot \Delta H) + \frac{\partial}{\partial \eta}(V\cdot \Delta H)\right) \tag{38}$$

where:

$$U = uy_\eta - vx_\eta, \tag{39}$$

$$V = vx_\xi - uy_\xi, \tag{40}$$

$$q_1 = x_\eta^2 + y_\eta^2, \tag{41}$$

$$q_2 = x_\xi x_\eta + y_\xi y_\eta, \tag{42}$$

$$q_3 = x_\xi^2 + y_\xi^2, \tag{43}$$

$$J = x_\xi y_\eta - x_\eta y_\xi. \tag{44}$$

Note that all improvements in this work are connected with flow prediction, whereas the simplest linear dependence of the liquid phase volume fraction on the temperature in a two-phase zone is employed. The usage of nonorthogonal coordinates and adaptive grids allow more accurate computations of heat and mass transfer at high Grashof numbers. A multiparametric investigation of dimensionless equations (35)–(44) at normal and reduced gravity conditions is conducted in this paper and refs. [89, 90] including buoyancy and thermocapillar convection.

The works considered in this paragraph indicate that numerical methods developed by different authors for solving convection/diffusion solidification problems and based on the 'porous medium' model can be generally interpreted from the mathematical viewpoint as a variant of fictitious regions methods.

5.2. *Stream function–vorticity formulation*

As for the fourth-order stream function equation for melt flow description, we recognize three basic variants of the fictitious regions method (see ref. [74] for more details). The first is based on the continuation of the coefficient at lower-order derivatives, the next approach uses the continuation of the coefficient at the second-order derivatives and the continuation of the coefficient at the fourth-order derivatives is carried out in the last variant. Only the first two variants can be found in the reviewed literature on mathematical modeling of convection/diffusion phase change processes.

In the first variant instead of equation (18) in the irregular domain $G^*(t)$ the following equation is to be solved in the whole domain G:

$$\frac{\partial \Delta\psi_\varepsilon}{\partial t} + (\mathbf{V}_\varepsilon, \operatorname{grad})\Delta\psi_\varepsilon = \operatorname{div}(\nu \operatorname{grad}\Delta\psi_\varepsilon) - C_\varepsilon\psi_\varepsilon + S_\varepsilon^\psi \tag{45}$$

where functions C_ε and S_ε^ψ are defined in just the same way as in (31), (32). This approach has been proposed in refs. [91, 92] for simulation of solidification in a cavity with hot and cold vertical walls. The same technique is applied in ref. [93] to predict metal solidification in a mould.

An example of the second variant of FRM is the method from ref. [94]. This variant can be considered as an extension of the 'porous medium' model approach in the stream function–vorticity formulation. In this case instead of equation (45) the following equation is to be solved:

$$\frac{\partial \Delta\psi_\varepsilon}{\partial t} + (\mathbf{V}_\varepsilon, \operatorname{grad})\Delta\psi_\varepsilon = \operatorname{div}(\nu \operatorname{grad}\Delta\psi_\varepsilon + C_\varepsilon \operatorname{grad}\psi_\varepsilon) + S_\varepsilon^\psi. \tag{46}$$

Note, that this variant of the fictitious regions method can be used to model incompressible viscous fluid flows in multi-connected domains.

5.3. *Flow prediction in the mushy region*

Mathematical models of heat and mass transfer processes in the mushy region can be based on various assumptions [95]. The emphasis here is on describing

mushy region processes and the inclusion of interactions between all existing zones. Starting with separate equations for each phase in the mushy region, authors carry out space averaging of these equations and derive unified continuous equations for the mushy region itself. This averaging can be done in different ways. To consider the mushy region as a liquid with solid inclusions, a variable viscosity model is used in some approaches. Another way is based on the 'porous medium' model and a dendritic structure assumption for the mushy region. Choosing one or another model it is useful to know the behavior of metal alloys in mushy region. The review [96] gives a good picture of the behavior of different alloys in some technological solidification processes.

To consider the mushy region as a porous medium (e.g. [97]), the momentum equation can be written as (29), (30), but the continuation coefficient C_ε and the RHS instead of (31), (32) are to be determined from some physical reasons based on the material properties. This approach has been used by different authors for modeling specific processes and fine agreement with experimental data has been obtained.

Let us list some applications of this method. Binary alloy solidification in a rectangular cavity is investigated numerically in ref. [98] in comparison with measurements. A comprehensive discussion of numerical methodologies for solving PDEs of the above mentioned model is done in ref. [99]. A mathematical model and its numerical implementation for prediction of the binary mixture NH_4Cl-H_2O melting is presented in ref. [100], where buoyancy-driven as well as surface-tension (Marangoni) convection are taken into account. An extended comparison between numerical and experimental results for this model can be found in ref. [101]. Numerical study of solidification of the binary solution Na_2CO_3 is conducted in ref. [102] for annuli between horizontal cylinders. It is interesting to point out an application of the above mentioned approach for phase change prediction in geology [103]. A similar 'porous medium' model has been used in ref. [104] for numerical simulation of convection/diffusion problems of melting. To increase the accuracy of computations on fixed rectangular grids, authors perform some correction of the coefficients in the vicinity of phase change interface for the energy equation using approximate analytical values for the thickness of the thermal boundary layer and the heat transfer coefficient.

Further developments of the mathematical model describing convection/diffusion phase change processes can be found in refs. [105, 106]. As distinct from the previous works, spatial variations of the liquid fraction are taken into account in this paper for the mushy region. This model also is based on the 'porous medium' assumption and unified equation formulation similar to (29), (30) for all phases—liquid, mushy and solid. Continuing the review of the works in this field, let us note the paper [107] where the model suggested in refs. [105, 106] is employed for the numerical simulation of vertical direct solidification of dendritic binary alloys.

In further studying convection/diffusion phase change processes and considering the mushy region, a hybrid model of the mushy region can be useful. Such a hybrid model based on some switching between the 'porous medium' model and the variable viscosity model depending on the solid fraction in the mushy region is developed in ref. [108].

6. CONCLUSIONS

Wide experience is accumulated in the numerical simulation of convection/diffusion phase change processes. Many groups of scientists are now developing numerical techniques for phenomena with phase change.

Most of the mathematical models are based on the conventional Boussinesq approximation for the Navier–Stokes equation. To improve the models, more correct hydrodynamics equations for the convective phenomena description are to be used. Further, it is necessary to consider more precisely processes in the vicinity of the phase change interface involving density variation through the interface. Note that in this case non-zero boundary conditions for the melt velocity have to be used at the phase change interface. New publications concerned with the mushy region model development can be expected.

Recapitulating all the above discussions, let us note once again that the numerical methods for solving convection/diffusion phase change problems can be divided into two different groups—variable grid methods and fixed grid methods. The fixed grid numerical methods are algorithmically more simple than variable grid techniques. For a long time there existed an opinion, that variable grid methods are more accurate, but Lacroix and Voller [109] demonstrated that the methods from the first and the second groups produced at the same order of mesh size practically identical solutions in sense of accuracy. From a mathematical point of view the fixed grid numerical methods can be considered as different variants of the fictitious regions method. Respectively, all accumulated results for this method such as existing, uniqueness and accuracy of the solution can be used in the mathematical modeling of convection/diffusion phase change problems.

It should be noted that there is a distance between modern computational mathematics and numerical methods for prediction convection/diffusion phase change. In some cases numerical techniques are employed without any theoretical validation of convergence, accuracy, etc. Unfortunately, it is impossible to obtain such validation for any problem that is to be solved numerically. But in cases where this validation is possible, it can be used for real decreasing of people's and computer's efforts in the numerical solution of these problems.

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