Int. J. Heat Mass Transfer. Vol. 35, No. 2, pp. 393–401, 1992
Printed in Great Britain

0017–9310/92 $5.00 + 0.00

Simulation of convective temperature oscillations in phase-change processes

J. PRAŽÁK†
Department of Physics, Czech. Tech. University, Thákurova 7, 16629 Prague 6, Czechoslovakia

and

J. PÁTEK
Institute of Thermomechanics, Czech. Acad. Sci., Dolejškova 5, 18200 Prague 8, Czechoslovakia

(*Received* 8 *April* 1990 *and in final form* 8 *October* 1990)

Abstract—This work is directed towards numerical simulations of short time temperature oscillations in liquid during the melting and/or solidification processes. A new approach based on the time-dependent Navier–Stokes equation developed for this purpose is proposed. The method is further applied to three example situations showing that it is capable of handling complicated phase-change problems. The mechanism of origin of the temperature oscillations in the vortices interaction is demonstrated.

1. INTRODUCTION

IN RECENT years, a number of various applications of solid–liquid phase changes have attracted considerable attention. Summarizing the work done in this field, we can say that experimental results advance slightly the theoretical description of the melting and/or solidification (M/S) processes. This can be explained by the fact that modelling of M/S processes includes modelling of two independent processes, each of which cannot be described generally in an analytic form:

(a) the natural convection in liquid;
(b) the evolution of the moving boundary of the solid–liquid interface.

The limitation of the description for the case where one of the two processes predominates is very often met in the approach to the modelling of M/S processes. We will briefly discuss approximations of this type.

The approach neglecting natural convection represents the direct development of the historical approach of Stefan [1]. It can provide us with a complex description of moving solid–liquid interfaces [2], but its application is limited to special cases such as a thin layer of a liquid or situations where forced convection plays the predominant role [3]. Modelling of this type can be improved by techniques accounting for natural convection in an approximative way, e.g. ref. [4].

Because of the importance of natural convection in M/S processes, the alternative approximative approach is the most frequently used, e.g. refs. [5–7]. This approach is based on the steady-state (time independent) Navier–Stokes equation. The time development of the solid–liquid interface is fully neglected or subsequently treated in an approximate way (the quasi-static approach). The steady-state description of natural convection gives realistic results for steady boundary conditions. For solving the free boundary problem, the finite element method with a suitably deformed grid is used. For the description of unsteady situations such as moving heater problems, this approach is sometimes used too [8]. However, the fact that the steady-state description does not depend on the latent heat of solidification, which is one of the governing quantites for processes of this type, limits the usefulness of this approximation.

For adequate description of M/S processes, the time-dependent Navier–Stokes equation seems to be necessary as the starting point. In combination with it, a 'quasi-static' approach to the moving solid–liquid interface leads to successful modelling of essentially non-stationary effects [9]. The approach presented in this paper gives yet more complete modelling with high time resolution within characteristic time intervals of temperature oscillations. It includes the complete time-dependent description of the interface by means of the weak formulation leading to the enthalpy methods [10, 11]. A suitable algorithm for the numerical treatment of the Navier–Stokes equation was constructed following ref. [12].

The most serious difficulty in computational fluid dynamics is the absence of mathematical results concerning the exact solutions of the Navier–Stokes equations. To overcome this, a special philosophy of a numerical (computational) experiment was formulated in ref. [13] and in yet more explicit form in ref. [14]. The main idea of this approach is expressed in the recommendation that the preparation of every

† Present address: Swiss Federal Institute of Technology Zürich, IBWK Hönggerberg, CH 8093 Zürich, Switzerland.

NOMENCLATURE

c	concentration on the admixed substance	ν	kinematic viscosity
D	diffusivity	ρ	density
g	gravitational acceleration	σ	rate of internal heat generation per unit volume
p	pressure	τ	time step
t	time	ψ	stream function
T	temperature	ω	vorticity.
T_0	temperature of phase change, temperature of reference		
$\mathbf{u}$	velocity	Subscripts	
$\mathbf{u}^*$	intermediate velocity.	A	top plate
		B	bottom plate
Greek symbols		L	liquid state
β	thermal expansion coefficient of liquid	n	concerning the time t
		$n+1$	concerning the time $t+\tau$
κ	thermal diffusivity	S	solid state.

computational code should be done in close parallel with the physical experiment and physical (experimental) argumentation should be used where the mathematical one is not available. In this paper, this type of numerical modelling is referred to as 'direct numerical simulation'.

The purpose of this paper is to present the direct numerical simulation of M/S processes with special attention to temperature oscillations in the liquid phase. Because of the considerable technological importance of such oscillations, we first mention some facts about them.

2. TEMPERATURE OSCILLATIONS IN M/S PROCESSES

Temperature oscillations in M/S processes are of great importance, especially in solidification processes (e.g. crystal growth), where they manifest themselves by oscillation of growth rate and lead to inhomogeneities of various types in the resulting solid material. Such material inhomogeneities are known as striations, e.g. refs. [15, 16].

The temperature oscillations observed in experiments [17, 18] differ in general by frequency spectrum, amplitude and attenuation [17, 18]. They arise from oscillatory or turbulent modes of two kinds of flows in liquid:

(a) buoyancy driven convection, if density gradients are present;

(b) thermocapillary (Marangoni) convection, if surface temperature gradients are present.

Buoyancy driven oscillations are studied both experimentally and theoretically in other processes too, e.g. in thermosyphons of various forms [19–21]. Interesting theoretical results were achieved by the interpretation of these oscillations in terms of the Lorenz attractor [22]. It seems to be natural that oscillations in melt material, at least some of them, can be interpreted in this way. However, it must be mentioned that a broad class of materials (those with a low Prandtl number, e.g. metals, silicon) does not have Prandtl numbers necessary for the occurrence of this phenomenon. The numerical modelling of the M/S processes for such cases therefore remains the most important tool for a theoretical analysis.

3. DIRECT SIMULATIONS OF M/S PROCESSES

The 'direct' approach to the simulation of M/S processes presented here was initially stimulated by the interest in the description of the floating zone (FZ) method of crystal growth (see ref. [23]), but the field of its application is rather more general.

The description starts from the Navier–Stokes equation

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\cdot\mathbf{u} = -\frac{\nabla p}{\rho} + \nu\Delta\mathbf{u} + \mathbf{g}\beta_L(T - T_0) \quad (1)$$

the continuity equation

$$\nabla\mathbf{u} = 0 \quad (2)$$

the equation of convective heat transfer

$$\frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T = \kappa_L\Delta T + \frac{\sigma}{\rho c} \quad (3)$$

and the equation of convective diffusion, if the migration of an admixed substance is to be studied

$$\frac{\partial c}{\partial t} + \mathbf{u}\cdot\nabla c = D_L\Delta c. \quad (4)$$

Equations (1)–(4) for the liquid part of the described system are completed by the equation of the conductive heat transfer for the solid part

$$\frac{\partial T}{\partial t} = \kappa_S \Delta T \tag{5}$$

and by the corresponding equation of diffusion

$$\frac{\partial c}{\partial t} = D_S \Delta c \tag{6}$$

if necessary.

Detailed kinetics of processes on the solid–liquid interface are to a considerable extent unknown. In fact, the direct simulation is a tool for the study of them. The description of this interface must be done with a high flexibility—various dependencies of the growing rate, such as dependence on undercooling, the shape of the interface, the position in the sample etc., must be considered. This can be done in the scope of the enthalpy concept—undercooling can be taken into account using the enthalpy—temperature dependence with a hysteresis loop, etc.

The numerical algorithm for solution of equations (1)–(6) has to be able to describe the observed temperature oscillations. Because of the high frequency of these oscillations (a typical measure of the generated striations is in the order of μm [16]), both the stationary and quasi-stationary approach are excluded.

The physical variables velocity–pressure $(\mathbf{u}, p)$ rather than the more usual stream function–vorticity (ψ, ω) make it possible to take into account various boundary conditions on both the moving and stationary boundaries in a physically adequate way. They are recommended for problems with a free boundary [13]. In addition, they make the description closer to the experiment.

The most serious step to conserve the high physical transparency and adaptability of the numerical simulation is the choice of a fully explicit scheme to calculate the values of the velocity and pressure fields at time t_{n+1} directly from the values at time t_n. In this context, 'directly' is meant as an opposite to the iterative and implicit way of ref. [12].

In fact, the fully explicit scheme is the most suitable tool for an analysis of the convective oscillations: it is known from experiments that a typical period can achieve values less than 1 s. In the simulations, a time step $\tau \sim 0.01$–0.1 s must therefore be used. It follows that the hard criterion limiting the time step for the explicit scheme does not influence the choice of τ seriously. On the other hand, solving the complete set of equations for an implicit scheme with the desired time frequency would lead to extreme time costs.

A well known difficulty in the numerical modelling of incompressible flows is the calculation of the pressure field $p(\mathbf{x}, t)$. Avoiding the iterative approach, we have adopted the method of intermediate velocity field recommended in ref. [14]. This method was inspired by dealing with compressible flows regarding the density as a variable quantity. The main idea consists of dividing the step calculating the velocity $\mathbf{u}_{n+1}$ on the basis of the velocity $\mathbf{u}_n$

$$\mathbf{u}_n \rightarrow \mathbf{u}_{n+1}$$

into two sub-steps

$$\mathbf{u}_n \underset{\text{I}}{\rightarrow} \mathbf{u}_n^* \underset{\text{II}}{\rightarrow} \mathbf{u}_{n+1}.$$

In sub-step I, the velocity field $\mathbf{u}_n^*$ is calculated according to the formula

$$\mathbf{u}_n^* = \mathbf{u}_n - [(\mathbf{u}_n \cdot \nabla) \cdot \mathbf{u}_n - \nu \Delta \mathbf{u}_n] \cdot \tau. \tag{7}$$

The velocity $\mathbf{u}^*$ is without physical meaning—it does not satisfy the continuity equation. It is corrected to a physical quantity in sub-step II

$$\mathbf{u}_{n+1} = \mathbf{u}_n^* - \frac{\tau}{\rho} \nabla p_{n+1}. \tag{8}$$

The pressure p in this relation is the solution of the Poisson equation

$$\Delta p_{n+1} = -\frac{\rho}{\tau} \nabla \cdot \mathbf{u}_n^*. \tag{9}$$

$\mathbf{u}_{n+1}$ satisfies both the Navier–Stokes and continuity equations, as can be verified.

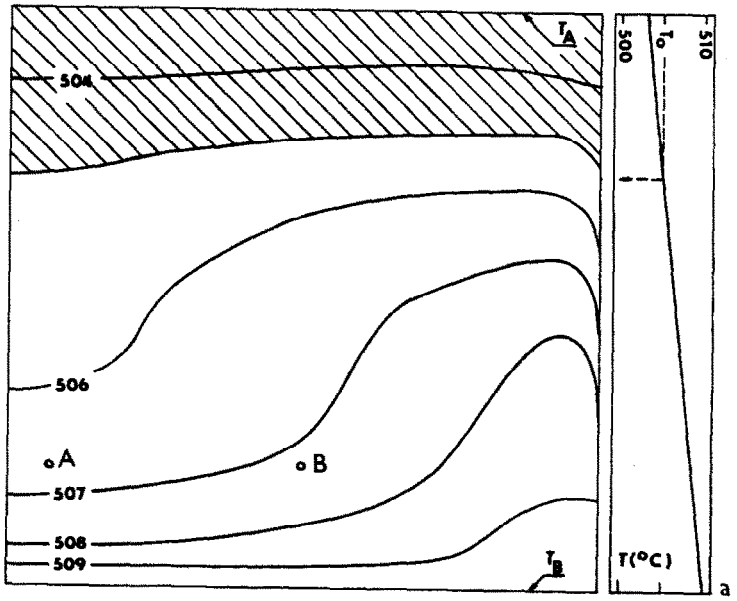
The described concept of the direct simulation of M/S processes was applied in the code ZONAL. Some results are presented in the next section.

4. EXAMPLES OF NUMERICAL RESULTS

In this section, the results of the numerical simulations of three experimental situations by the code ZONAL are presented. The temperature oscillations during the M/S processes were studied. Because of the fact that only the general possibility of occurrence of the oscillations was of interest, the hypothetical materials were used: in the set of material characteristics corresponding to tin (Sn), the latent heat was changed to accelerate/retard time development of the solid–liquid interface.

Example I

The development of the solid–liquid interface in a cylindrical sample 2 cm in height and 2 cm in radius was simulated. The initial state was characterized by the homogeneous temperature distribution at the freezing point of the material ($T_0 = 505$°C) and the planar horizontal solid–liquid interface at 5/7 the height above the bottom. The temperature changing linearly from $T_A = 503$°C at the top to $T_B = 507$°C at the bottom, was applied on the outside of the sample at the initial moment. The resultant steady shapes of the solid–liquid interface with the temperature field (T) and the velocity field (ψ) in one half of the planar section are displayed in Figs. 1(a) and 1(b) respectively. Transient temperature oscillations monitored during the simulation in points denoted as A and B are shown in Fig. 2.



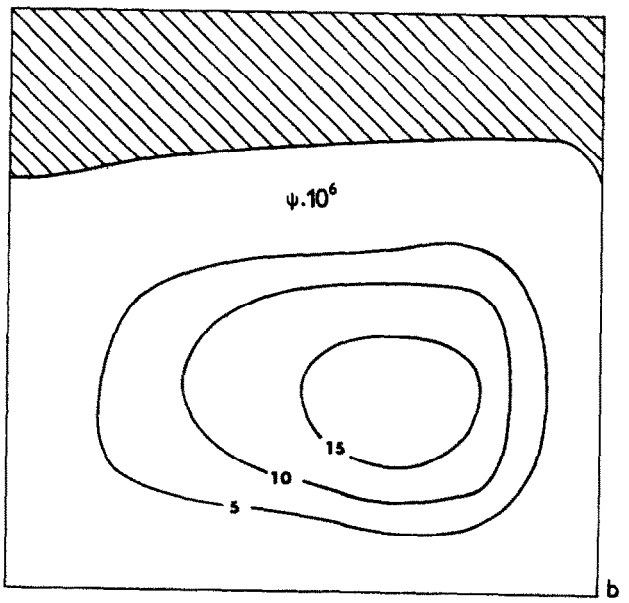


FIG. 1. Resultant steady shape of the solid–liquid interface in one half of the planar section of the cylindrical sample heated from below and the corresponding temperature field (a) and stream function (b). The axis of the sample lays on the left; A and B are the points where the temperature is monitored (see Fig. 2).

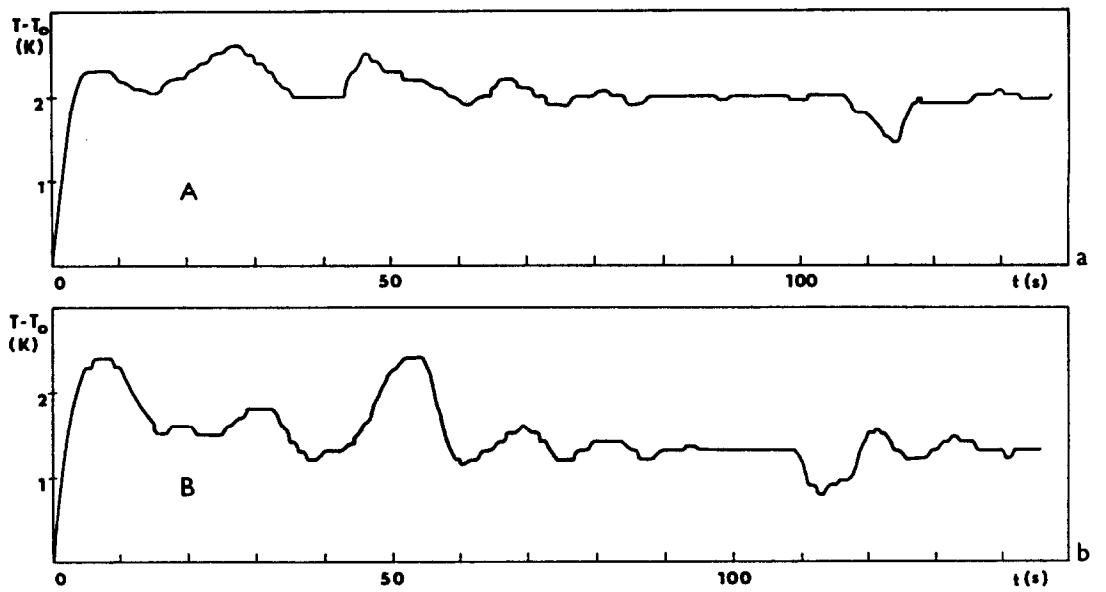


FIG. 2. The development of the temperature in the points denoted at A and B in Fig. 1.

Example II

The development of the solid–liquid interface during melting from below is presented in Fig. 3 ($T_B = 520°C$, $T_A = 500°C$). In contrast to the preceding example, pronounced temperature oscillations can be registered in the liquid (Fig. 4). It is interesting to compare these results with experimental work [17].

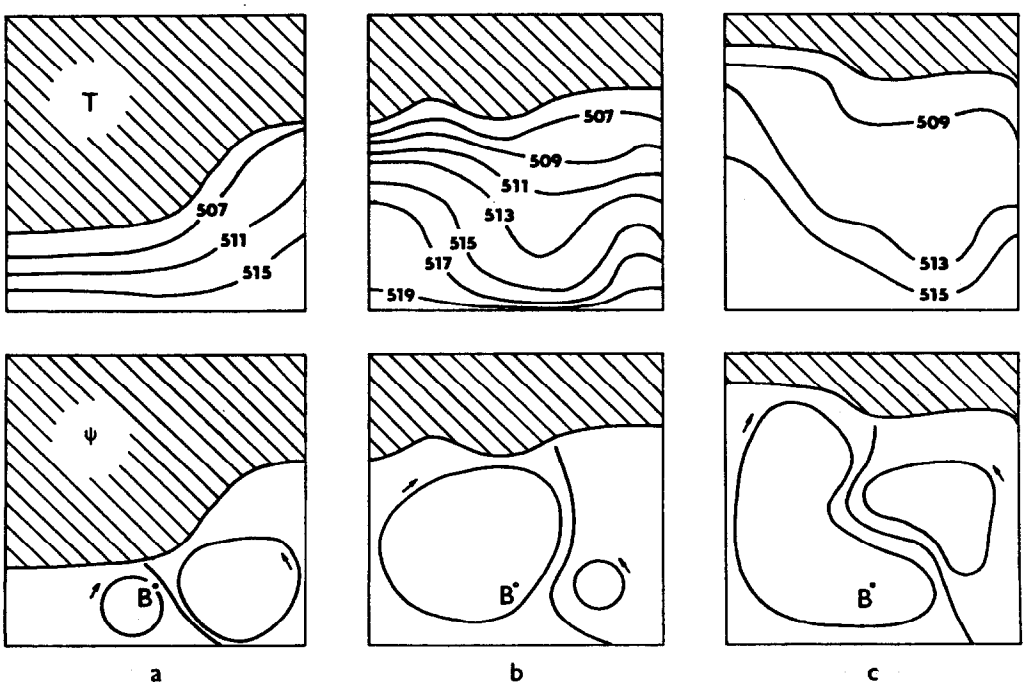


FIG. 3. The development of the temperature, streaming and solid–liquid interface in a sample 2 cm in height and 2 cm in radius during its melting from below. Situations at times 7.5, 37.5 and 60 s are displayed in (a), (b) and (c), respectively. B is the point where the temperature is monitored (see Fig. 4).

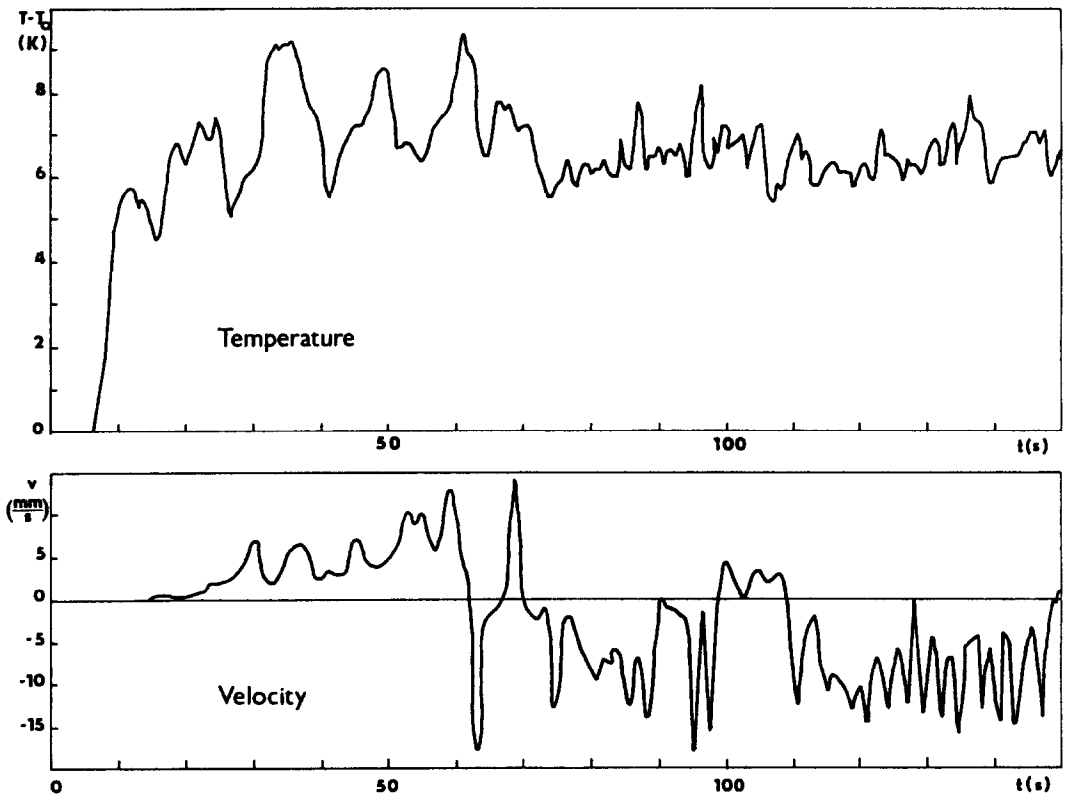


FIG. 4. The temperature and horizontal velocity component fluctuations at the point denoted as B in Fig. 3.

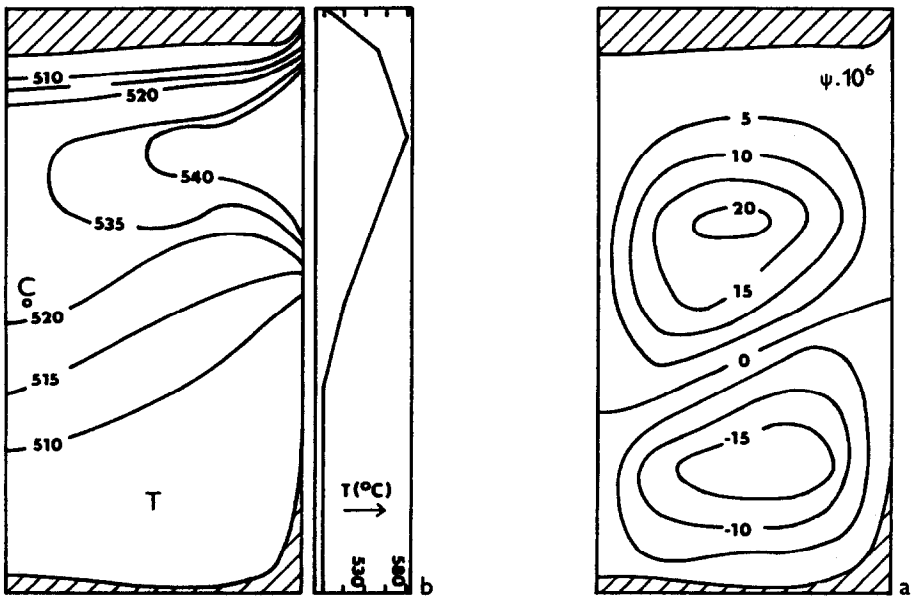


FIG. 5. Modelling of the situation arising by the floating zone (FZ) crystal growth method in a cylindrical sample 2.8 cm in height and 1.7 cm in radius. The temperature applied on the sample from the side is displayed on the right of (a). C is the point where the temperature is monitored (see Fig. 6).

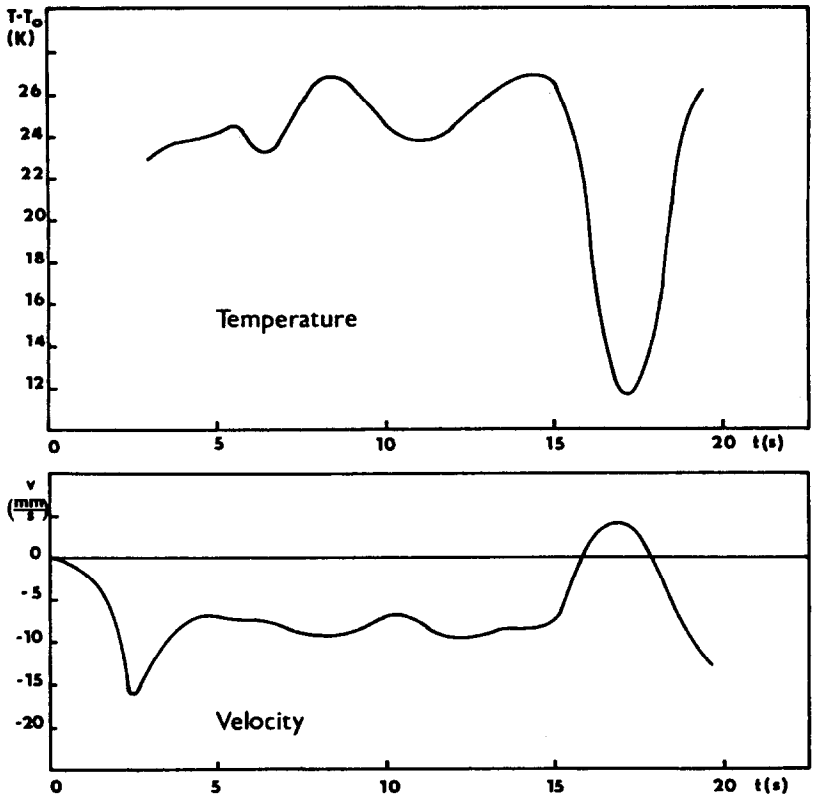


FIG. 6. The temperature and vertical velocity component oscillations in the point denoted as C in Fig. 5.

Example III

The situation displayed in Fig. 5 represents the one arising by the FZ method of crystal growth. The significant temperature oscillations (Fig. 6) can be explained by the interaction of the two vortices present in the liquid (see Fig. 7).

5. CONCLUSION

The main features of the direct approach to simulation of M/S processes are the use of physical variables, the enthalpy concept of description of phase changes and the fully explicit scheme for solving the

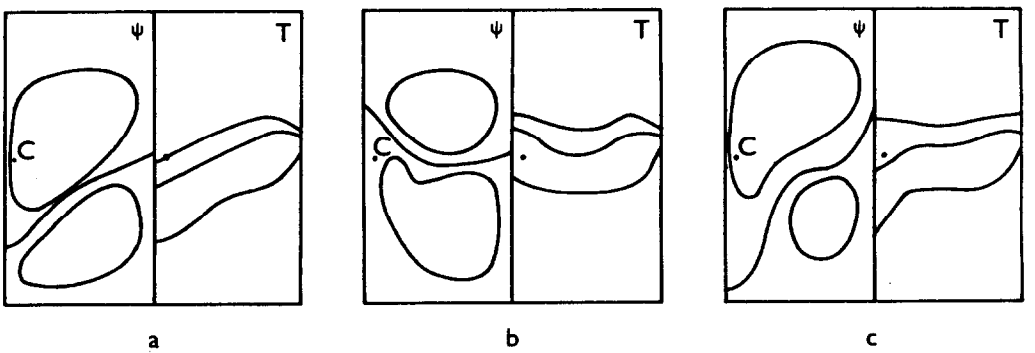


FIG. 7. The mechanism of the temperature oscillations registered in point C (Fig. 5): during 4.5 s, the position of the two vortices present in the liquid changes essentially relative to point C. (a) 15 s; (b) 17.5 s; (c) 19.5 s.

transport equations. This approach seems to be very fruitful for these tasks, where the physical nature of the experimentally observed oscillatory behaviour is to be investigated. The adaptability of corresponding codes facilitates the development of the physical picture laying in its base.

The Boussinesq approximation used in equations (1)–(4) is characterized by the extreme simplicity in handling the equation of state of the liquid. It is quite suitable in the bulk liquid. At the phase interface, the described approach also allows us to modify the starting approximation. A description using a more complex equation of state for the liquid can be used, if it appears to be useful.

On the other hand, it should be mentioned that the direct simulation is designed for physical research computations rather than for serial ones: the conservation of maximal adaptability makes to a certain degree undesirable and/or impossible the optimization from the point of view of the efficiency of the corresponding codes. The flexibility is therefore at the expense of increased time costs, especially in cases where no oscillations occur.

Acknowledgement—This work was supported in part by a contract from the INTERCOSMOS Research Program.

REFERENCES

1. J. Stefan, Ueber die Theorie der Eisbildung, insbesondere ueber die Eisbildung in Polarmeeren, *Ann. Phys. Chem.* **42**, 269–286 (1891).
2. Y. Cao, A. Faghri and W. S. Chang, A numerical analysis of Stefan problems for generalized multi-dimensional phase-change structures using the enthalpy transforming model, *Int. J. Heat Mass Transfer* **32**, 1289–1298 (1989).
3. S. E. Hibbert, N. C. Markatos and V. R. Voller, Computer simulation of moving-interface, convective, phase-change processes, *Int. J. Heat Mass Transfer* **31**, 1785–1795 (1988).
4. Z. Zhang and A. Bejan, Melting in an enclosure heated at constant rate, *Int. J. Heat Mass Transfer* **32**, 1063–1076 (1989).
5. C. J. Chang and R. A. Brown, Finite element calculation of buoyancy-driven convection near a melt/solid phase boundary. In *Numerical Properties and Methodologies in Heat Transfer, Proc. Second Natn. Symp.* (Edited by T. M. Shih), p. 283. Hemisphere, Washington, DC (1981).
6. C. Bernard, D. Gobin and A. Zanoli, Moving boundary problem: heat conduction in the solid phase of a phase-change material during melting driven by natural convection in the liquid, *Int. J. Heat Mass Transfer* **29**, 1669–1681 (1986).
7. J. L. Duranceau and R. A. Brown, Thermal-capillary analysis of small-scale floating zones: steady-state calculations, *J. Crystal Growth* **75**, 367–389 (1986).
8. B. Basu and J. Srinivasan, Numerical study of laser melting problem, *Int. J. Heat Mass Transfer* **31**, 2331–2338 (1988).
9. M. E. Thompson and J. Szekely, Density stratification due to counterbuoyant flow along a vertical crystallization front, *Int. J. Heat Mass Transfer* **32**, 1021–1036 (1989).
10. V. R. Voller and C. Prakash, A fixed grid numerical modelling methodology for convection–diffusion mushy region phase-change problems, *Int. J. Heat Mass Transfer* **30**, 1709–1719 (1987).
11. C. Prakash, M. Samonds and A. K. Singhal, A fixed grid numerical methodology for phase change problems involving a moving heat source, *Int. J. Heat Mass Transfer* **30**, 2690–2694 (1987).
12. S. V. Pantankar, *Numerical Heat Transfer and Fluid Flow*. Hemisphere, Washington, DC (1980).
13. P. J. Roache, *Computational Fluid Dynamics*. Hermosa, Albuquerque (1976).
14. O. M. Belocerkovskij, *Numerical Modelling in Continuum Mechanics*. Nauka, Moscow (1984) (in Russian).
15. T. Carlberg, Some aspects of the formation of striations during crystal growth from the melt, *J. Crystal Growth* **85**, 32–39 (1987).
16. A. Eyer, H. Leiste and R. Nitsche, Floating zone growth of silicon under microgravity in a sounding rocket, *J. Crystal Growth* **71**, 173–183 (1985).
17. K. Kamotani and J. Kim, Effect of zone rotation on oscillatory thermocapillary flow in simulated floating zones, *J. Crystal Growth* **87**, 62–68 (1988).
18. G. Gau and R. Viskanta, Melting and solidification of a metal system in a rectangular cavity, *Int. J. Heat Mass Transfer* **27**, 113–123 (1984).
19. J. E. Hart, Observations of complex oscillations in a closed thermosyphon, *J. Heat Transfer* **107**, 833–839 (1985).
20. G. S. H. Lock and Y. Liu, The effect of geometry on the performance of the closed tube thermosyphon at low Rayleigh numbers, *Int. J. Heat Mass Transfer* **32**, 1175–1182 (1989).
21. K. Chen, On the oscillatory instability of closed loop thermosyphons, *J. Heat Transfer* **107**, 826–832 (1985).
22. J. E. Hart, A new analysis of the closed loop thermosyphon, *Int. J. Heat Mass Transfer* **27**, 125–136 (1984).
23. V. A. Tatarcenko, *Stationary Crystal Growth*. Nauka, Moscow (1988) (in Russian).

SIMULATION DES OSCILLATIONS DE TEMPERATURE CONVECTIVE DANS DES MECANISMES DE CHANGEMENT DE PHASE

Résumé—On étudie par simulation numérique les oscillations rapides de température dans un liquide pendant les mécanismes de fusion et/ou de solidification. On propose une nouvelle approche basée sur l'équation de Navier–Stokes dépendant du temps et développée dans ce but. La méthode est appliquée ensuite à trois exemples montrant qu'elle est capable de traiter des problèmes compliqués de changement de phase. On traite du mécanisme des oscillations de température dans l'interaction des tourbillons.

SIMULATION KONVEKTIVER TEMPERATURSCHWINGUNGEN BEI PHASENWECHSELVORGÄNGEN

Zusammenfassung—Es wird die numerische Simulation von hochfrequenten Temperaturschwingungen in Flüssigkeiten während des Schmelz- und/oder Erstarrungsvorgangs beschrieben. Hierfür wird ein auf der zeitabhängigen Navier–Stokes-Gleichung basierender neuer Ansatz entwickelt. Die Methode wird auf drei Beispiele angewandt, um aufzuzeigen, daß die Behandlung komplizierter Phasenwechselprobleme möglich ist. Es wird gezeigt, daß die Temperaturschwingungen durch Wirbelwechselwirkungen entstehen.

МОДЕЛИРОВАНИЕ КОЛЕБАНИЙ ТЕМПЕРАТУР В ПРОЦЕССАХ КОНВЕКТИВНОГО ТЕПЛООБМЕНА С ФАЗОВЫМ ПЕРЕХОДОМ

Аннотация—Численно моделируются колебания температуры жидкости в процессах плавления и (или) затвердевания. Предложен новый подход на основе нестационарного уравнения Навье–Стокса. Этот метод далее иллюстрируется на трех примерах, при этом показано, что он может успешно использоваться для решения сложных задач фазового перехода. Описывается механизм возникновения температурных колебаний при взаимодействии вихрей.