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Boundary control of the medium motion in problems of crystallization and melting

by

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As it is well known, the motion equations of a continuum written as conservation laws of mass, momentum and energy have a divergent form. Thus a generalized motion can be defined which admits discontinuities of motion characteristics such as velocity, density, specific internal energy and stress. If the medium characteristics of the generalized motion exhibit discontinuity along some hypersurface Γ_T and have a necessary number of derivatives everywhere beyond Γ_T, the generalized motion is called the strong discontinuity motion.

As examples of such a motion one can take in particular shock waves in gas dynamics or phase transitions in a pure matter described by a classical solution of Stefan problem.

The goal of this work is to construct simple closed mathematical models of phase transitions which take into account a medium motion. One--dimensional motions with plane waves are the simplest among them.

Let Ω be a domain in Lagrange variables (x, t) where functions J (specific volume), u (velocity), P (stress), V (specific internal energy) and θ (temperature) to be determined satisfy the system of equations

$$\frac{\partial J}{\partial t}=\frac{\partial u}{\partial x}, \frac{\partial u}{\partial t}=\frac{\partial P}{\partial x}, \tag{1}$$

$$\frac{\partial}{\partial t}\left(\frac{1}{2}u^2+V\right)=\frac{\partial}{\partial x}\left(\frac{\varkappa}{J}\cdot\frac{\partial\theta}{\partial x}+Pu\right) \tag{2}$$

in the distribution sense.

These equations are to be satisfied along with the following state equations

$$P = \frac{\mu}{J} \cdot \frac{\partial u}{\partial x} - p_0(\theta, J), \theta = \chi(V). \tag{3}$$

Let us assume from now on that the melting temperature of the medium is constant. Without loss of generality it can be assumed to be equal zero. If $\chi(V) > 0$ for $V > 0$, $\chi(V) = 0$ for $V \in [-L, 0]$, $\chi(V) < 0$ for $V < -L$ and $\chi'(V) > 0$ for $V \notin [-L, 0]$, then the second equation in (3) defines a liquid ($V \geqq 0$), solid ($V \leqq -L$) and mushy ($-L < V < 0$) region of the medium [1].

In the case of a strong discontinuity motion in the crystallization or melting problems, there exists a finite number of the smooth curves $\Gamma_T = \{(x, t) | x = R(t), t \in (0, T)\}$ in $\Omega_T = \Omega \times (0, T)$. Upon crossing them, the medium characteristics (maybe, not all of them) undergo discontinuities of the first kind, and everywhere beyond those curves they satisfy the differential equations (1), (2) in the classical sense.

On the phase transition curves Γ_T the limit values of the unknown functions are not arbitrary but have to satisfy the conditions of the strong discontinuity:

$$[J] \cdot \frac{dR}{dt} + [u] = 0, [u] \cdot \frac{dR}{dt} + [P] = 0, \tag{4}$$

$$\left[\frac{1}{2} u^2 + V\right] \cdot \frac{dR}{dt} + \left[\frac{\varkappa}{J} \cdot \frac{\partial \theta}{\partial x} + Pu\right] = 0. \tag{5}$$

Before embarking upon the analysis of (4), (5), it seems reasonable to introduce some simplifying assumptions. First, let us ignore the energy dissipation in the heat equation (2) and write it down as

$$\frac{\partial V}{\partial t} = \frac{\partial}{\partial x}\left(\frac{\varkappa}{J} \cdot \frac{\partial \theta}{\partial x}\right).$$

This is related to the fact that even in the universally accepted Stefan problem for a nonhomogeneous heat equation the conditions under which the generalized solution is in the form of the strong discontinuity motion have not been clarified up to now.

Provided the heat equation is homogeneous, there is no transient phase at an initial time moment, and the liquid and solid phases consist of a finite number of connected components, in the case of one space variable the generalized solution of the Stefan problem is the classical one, therefore it represents a strong discontinuity motion. An analogous structure is to be expected for the solution in more complicated situations.

According to the heat equation, the strong discontinuity condition takes the form:

$$[V]\cdot\frac{dR}{dt}+\left[\frac{\varkappa}{J}\cdot\frac{\partial\theta}{\partial x}\right]=0. \tag{6}$$

In the sequel we shall assume that in the domain Ω_T there is only one strong discontinuity interface Γ_T (free surface) between the liquid and solid phases, and one of the phases has temperature equal to the melting temperature.

Let us consider two cases:

(A) In liquid and solid states the medium is viscous, i.e.

$$P=\frac{\mu}{J}\,\frac{\partial u}{\partial x},\ \mu=\text{const}>0 \qquad \text{for } \theta>0,$$

$$P=-p_0(\theta, J)+\frac{\mu_s}{J}\cdot\frac{\partial u}{\partial x},\ \mu_s=\text{const}>0 \text{ for } \theta<0,$$

the liquid phase occupies the domain $\Omega_T^+=\{(x,t)|0<x<R(t),\ 0<t<T\}$, the solid occupies $\Omega_T^-=\{(x,t)|x>R(t),\ 0<t<T\}$ and has zero temperature; besides, on the boundary $x=0$ the heat flow and stress are equal to zero.

(B) In the solid state the medium has elastic properties, i.e.

$$P=-\gamma\cdot\theta+\beta\cdot J,\ \beta=\text{const}>0 \text{ for } \theta<0;$$

the solid phase occupies the domain $\Omega_T^-=\{(x,t)|R(t)<x<1,\ 0<t<T\}$, on the boundary $x=1$ the velocity and heat flow are equal to zero, and in the liquid phase which occupies the domain $\Omega_T^+=\{(x,t)|x<R(t),\ 0<t<T\}$ the temperature is equal to that of melting.

In the case (A), the first equation of (3) can be treated as the differential equation

$$\frac{\partial u}{\partial x}=\frac{J}{\mu(\theta)}\cdot(P+p_0(\theta,J)) \text{ in } \Omega_T,$$

which yields the strong discontinuity condition

$$[u]=0 \text{ on } \Gamma_T.$$

This condition, together with (4), implies that the specific volume J and the stress P are continuous on the strong discontinuity line Γ_T.

Generally speaking, stresses and displacements in the solid phase differ from zero and effect convection in the liquid phase.

There are two ways of constructing the solutions to the above problem. The first one consists in solving the equations of motion over the domain Ω_T^- that is rather complicated procedure. The other one is to assume that the density of the solid phase is equal to a certain known constant and therefore the equations of motion throughout Ω_T^- can be neglected. However, in order to determine correctly the solution in Ω_T^+ and the proper domain Ω_T^+ itself, it is necessary to specify additionally either the velocity, stress or some value related to them on the free surface. Since it is definitely impossible to determine all these values, one should postulate that an additional information is available, e.g. the specific volume in the liquid phase is at the moment of complection of the process close to a known constant J_L.

Prior to giving an effective formulation of the problem (A), let us transform it to a more convenient form. By differentiation of the equations (1) with the subsequent integration in time, one gets the following equation for the function $\omega = \ln J$:

$$e^{\omega}\cdot\frac{\partial\omega}{\partial t} = \frac{\partial^2\omega}{\partial x^2} + f(x),\ (x, t)\in\Omega_T^+, \tag{7}$$

where $f(x) = 0$ at $x \in (0, R_0)$ and it is to be determined at $x \geqq R_0$. The function $f(x)$ represents the influence of the solid phase onto liquid one and can be determined from an additional information by minimization of a relevant functional. Since the time derivative of the function ω on the boundary $x = 0$ is equal to zero (by the equation and due to condition that the stress on the boundary $x = 0$ is equal to zero), ω is constant on this boundary, also

$$\omega(0, t) = \omega_0(t),\ t\in(0, T) \tag{8}$$

Problem (A): Summing up, we have arrived at the following formulation. Determine the domain Ω_T^+ and functions ω, θ, V, f which satisfy the system consisting of (7), (8) and

$$\frac{\partial V}{\partial t} = \frac{\partial}{\partial x}\left(\varkappa e^{-\omega}\cdot\frac{\partial\theta}{\partial x}\right),\ \theta = \chi(V),\ (x, t)\in\Omega_T^+, \tag{9}$$

$$\frac{\partial\theta}{\partial x} = 0,\ x = 0,\ t\in(0, T), \tag{10}$$

$$\theta = 0,\ \omega = \mathring{\omega},\ x = R(t),\ t\in(0, T), \tag{11}$$

$$L\frac{dR}{dt} = -\varkappa e^{-\omega}\cdot\frac{\partial\theta}{\partial x},\ x = R(t),\ t\in(0, T), \tag{12}$$

$$R = R_0,\ \theta = \theta_0(x),\ \omega = \omega_0(x)\ \text{at}\ t = 0,\ x\in(0, R_0), \tag{13}$$

where L, $\mathring{\omega}$, μ, $\varkappa$, $R_0 = \text{const} > 0$.

The unknown function $f(x)$ is to be determined by the minimization of the functional

$$\Psi_0(f) = \int_0^{R(T)} |J(x, T) - J_L|^2\, dx. \tag{14}$$

In the case (*B*) the first equation in (3) is degenerate, i.e. the viscosity coefficient μ equals zero in the solid phase. Consequently, the velocity, density and stress can exhibit the first kind discontinuity on the free surface.

By an analysis of the structure of the problem in the case (*B*), it follows that in order to determine the domain Ω_T^- and the characteristics of its motion without solving the corresponding equations of motion in the liquid phase, one needs to know either the velocity or specific volume along the free surface, together with the relevant initial conditions, the conditions on the fixed boundary $x = 1$:

$$\frac{\partial J}{\partial x} = 0,\ \frac{\partial \theta}{\partial x} = 0,\ x = 1,\ t \in (0, T), \tag{15}$$

as well as to prescribe the Stefan condition (6) and equality of the temperature on the free surface to zero.

Just as in the case (*A*), it is impossible to determine directly the above-mentioned values, therefore they are to be found via a functional minimization analogous to (14).

In Ω_T^-, the specific volume J satisfies the nonhomogeneous wave equation

$$\frac{\partial^2 J}{\partial t^2} = \beta \frac{\partial^2 J}{\partial x^2} - \gamma \frac{\partial^2 \theta}{\partial x^2},\ (x, t) \in \Omega_T^-. \tag{16}$$

If the velocity of the free boundary is small, only one family of characteristics originate from this line. In this case, an additional boundary condition may be prescribed on the known boundary $x = 1$:

$$J = \mathring{J}(t),\ x = 1,\ t \in (0, T). \tag{17}$$

Now we can give an accurate formulation in the case (*B*).

Problem (*B*): Determine a function $R(t)$ which defines the domain Ω_T^- and functions J, u, θ, V satisfying in Ω_T^- equations (9), (16), boundary conditions (12), (15), (17) and the conditions

$$\theta = 0,\ x = R(t),\ t \in (0, T), \tag{18}$$

$$R = R_0,\ \theta = \theta_0(x),\ J = J_0(x),\ \frac{\partial J}{\partial t} = 0,\ x \in (R_0, 1). \tag{19}$$

The unknown function $\mathring{J}(t)$ is to be determined by minimization of the functional

$$F_0(\mathring{J}) = \int_{R(T)}^{1} |J(x, T) - J_s|^2 \, dx. \tag{20}$$

Using methods standard for the analysis of second-order parabolic equations, it can be shown that the set of those $f(x)$ for which the problem (7)–(13) has a unique solution is not empty.

THEOREM 1. *Let* $V = c_L \cdot \theta$, $c_L = \text{const} > 0$, L, $\varkappa$, μ, $\mathring{\omega}$, $R_0 = \text{const} > 0$, θ_0, $\omega_0 \in C^2[0, R_0]$, $f \in L_2[0, X]$, where $X \geqq R_0 + \frac{1}{L}\int_0^{R_0} \theta_0(x)\,dx$. *Then the problem* (7)–(13) *has a unique solution* R, ω, V, θ *such that* $\omega, \theta \in W_2^{2,1}(\Omega_T^+)$, $R \in H^{1+\gamma}[0, T]$.

As it is well known, the less information is contained in the functional (14), the more difficult is to determine its minimum. For that reason in this work we will specify the function $f(x)$ as a minimizer of the functional

$$\Psi(f) = \Psi_0(f) + \alpha \|f\|^2_{L_2[0,X]}, \tag{21}$$

where $\alpha > 0$ is a sufficiently small number.

THEOREM 2. *Under the assumptions of Theorem 1, there exists at least one element f of $L_2[0, X]$ which minimizes the functional* (21).

Analogous results are true for the problem (*B*), but in contrast to (*A*) we are unable to provide strict positivity of the specific volume J throughout the domain Ω_T^-. Thus in a proof of the assertion analogous to Theorem 1, it is necessary to demand a smallness of the initial temeprature $\theta_0(x)$.

References

[1] MEIRMANOV A. M. Structure of generalized solution of Stefan problem. Periodical solutions. *Dokl. Akad. Nauk SSSR*, **272**, (1983) 4, 789–892.

Sterowanie brzegowe ruchu ośrodka w problemach krystalizacji i topnienia

Praca dotyczy konstrukcji i analizy modeli matematycznych procesów fazowych, sformułowanych w terminach ruchu uogólnionego. Ruch ten charakteryzuje się nieciągłością charakterystyk takich jak szybkość przepływu, gęstość, energia wewnętrzna i naprężenie. Rozważane są dwa modele odpowiadające założeniom o lepkości lub elastyczności ośrodka. Proponowane modele mają postać zamkniętego układu równań różniczkowych cząstkowych związanego z pewnym zadaniem minimalizacji funkcjonału. Podane są twierdzenia o istnieniu i jednoznaczności rozwiązań modeli.

Граничное управление в проблемах кристаллизации и плавления относительно движения среды

Предметом работы является конструкция и анализ математических моделей для процессов фазовых переходов относительно обобщённого движения, которое характеризуется непрерывностями таких характеристик как скорость, плотность, внутренняя энергия в напряжение. Предлагаются две модели соответствующие предположениям о вязкости либо упругости среды. Модели имеют вид замкнутой системы дифференциальных уравнений в частных производных связанной с некоторой задачей манимизации функционала. Сформулированы теоремы о существовании и единственности решений.