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MATHEMATICAL AND NUMERICAL BASIS OF BINARY ALLOY SOLIDIFICATION MODELS WITH SUBSTITUTE THERMAL CAPACITY. PART I

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Abstract. The presented work is focused on the basis of mathematical and numerical descriptions of the binary alloy solidification problem. The mathematical formulation is based on the so-called substitute thermal capacity, which implies a change in the specific heat of solidifying material. In the literature one can find many ways to define this parameter. Five models, differing in the description of the substitute thermal capacity as well as the numerical model using the finite element method (FEM) are considered.

Keywords: *solidification, substitute thermal capacity, modeling, finite element method*

Introduction

Solidifying alloy is a complex system of related physical processes taking place in the same time from nano- to macroscale. The formation process of the casting can be divided into four main phases:

- The pouring phase when the molten material is introduced into the mold. The phase is accompanied by intense mixing occurring mainly as a result of forced convection.
- Cooling in the liquid state phase when the forced convection of the liquid gradually disappears giving way to movement caused by the phenomenon of natural convection, the intensity of which is determined by the degree of change in density of the material caused by changes in temperature.
- The solidification phase, which is characterized by solid phase growth. The process of liquid-solid phase transformation is egzoenergetic, accompanied by release of heat to the surrounding area.
- Cooling in the solid state phase during which the temperature of the casting is lowered to a value which allows removing it from the mold and carry out the final treatment.

The most important stage in the formation of casting is the solidification phase since it determines the structure and quality of the final product. Numerical model-

ing of this process has been a widely discussed problem for many years in the literature. The key task of the creator of the numerical model is an appropriate description of the process of the heat emission and transport in the solidifying area. In the case of binary alloys so-called models with substitute thermal capacity are often used [1-4]. The models based on the enthalpy [5, 6] are very popular either.

1. Mathematical model

The binary alloy solidification problem in the two-dimensional region is considered. Solid phase appears on the cooled boundary when the temperature drops below the liquidus temperature T_L and it coexists with the liquid phase until the temperature reaches the solidus temperature T_S. Participation of the solid phase is a dimensionless parameter f_s from the interval [0, 1]. There are three zones in the analyzed region, where Ω_S contains solid, Ω_L is filled with liquid while Ω_{S+L} is a mixture of phases. The boundaries between them coincide with solidus and liquidus isotherms (Fig. 1).

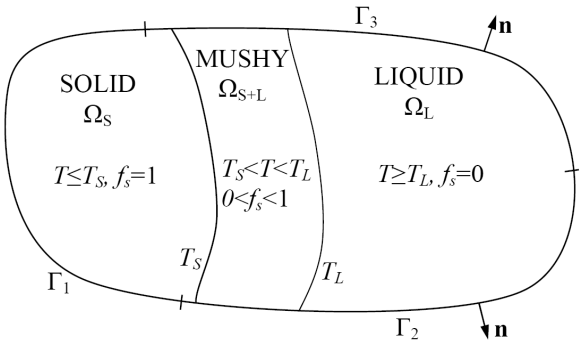

Fig. 1. Subregions in the considered problem

The basis of the mathematical description of the problem is the equation of energy (1), where the classical heat diffusion equation is supplemented by a source term which describes heat emission during solidification:

$$\frac{\partial}{\partial x}\left(\lambda_m \frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda_m \frac{\partial T}{\partial y}\right)+\rho_s L\frac{\partial f_s}{\partial t}=\rho_m c_m \frac{\partial T}{\partial t} \tag{1}$$

where T [K] denotes temperature, c_m [J/(kgK)] is averaged specific heat, ρ_m [kg/m^3] - averaged density, λ_m [W/(mK)] - averaged coefficient of thermal conductivity, L [J/kg] - latent heat of solidification, t [s] - time, s - index referring to solid.

Averaging of material parameters is carried out using the parameter f_s:

$$\lambda_m = f_s\lambda_s+(1-f_s)\lambda_l,\quad \rho_m = f_s\rho_s+(1-f_s)\rho_l,\quad c_m = f_s c_s+(1-f_s)c_l \tag{2}$$

Participation of the solid phase is a function of the temperature and indirectly of time $f_s = f_s(T)$, therefore equation (1) can be written in the following form:

$$\frac{\partial}{\partial x}\left(\lambda_m \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda_m \frac{\partial T}{\partial y}\right) = \rho_m c_m \frac{\partial T}{\partial t} - \rho_s L \frac{df_s}{dT}\frac{\partial T}{\partial t} \tag{3}$$

$$\frac{\partial}{\partial x}\left(\lambda_m \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda_m \frac{\partial T}{\partial y}\right) = \left(\rho_m c_m - \rho_s L \frac{df_s}{dT}\right)\frac{\partial T}{\partial t} \tag{4}$$

By introducing simplification through the adoption of solid density ρ_s equal to the average density of the mushy zone ρ_m substitute thermal capacity is obtained:

$$c_{eff} = c_m - L\frac{df_s}{dT} \tag{5}$$

Equation (4) can then be rewritten in the form shown below

$$\frac{\partial}{\partial x}\left(\lambda_m \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda_m \frac{\partial T}{\partial y}\right) = \rho_m c_{eff} \frac{\partial T}{\partial t} \tag{6}$$

Equation (6) shall be complemented by the appropriate boundary and initial conditions:

$$\Gamma_1 : T = T_b \tag{7}$$

$$\Gamma_2 : -\lambda \frac{\partial T}{\partial n} = -\lambda \nabla T \cdot \mathbf{n} = q_b \tag{8}$$

$$\Gamma_3 : -\lambda \frac{\partial T}{\partial n} = \alpha\left(T - T_\infty\right) \tag{9}$$

$$T\left(t = 0\right) = T_0 \tag{10}$$

where T_b [K] is known temperature on the boundary Γ_1, q_b [W/m^2] - known heat flux through the boundary Γ_2, $\partial T/\partial n$ - directional derivative of temperature, $\mathbf{n}$ - vector normal to the boundary Γ_2, α [W/(m^{2}K)] - convective heat transfer coefficient, T_∞ [K] - ambient temperature, T_0 [K] - initial temperature.

Equation (6) with the boundary conditions (7)-(9) and the initial condition (10) are the basis of the mathematical model of the solidification problem. There are several methods for calculating $c_{eff}(T)$ [1, 3]. Assuming a linear distribution $f_s(T)$ in the temperature range $[T_S, T_L]$, a constant value of substitute thermal capacity is obtained (Fig. 2a):

$$c_{eff}(T) = c_m + \frac{L}{T_L - T_S} \tag{11}$$

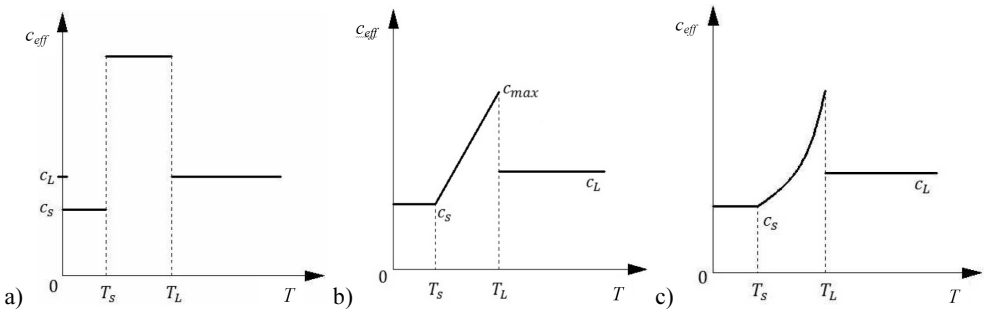

Fig. 2. Distribution of c_{eff} for hypothesis 1-3

Assuming a linear distribution c_{eff} (Fig. 2b) the following expression is used:

$$c_{eff}(T) = c_s + (c_{\max} - c_s)\frac{T - T_S}{T_L - T_S} \tag{12}$$

where the parameter $c_{\max}$ can be determined from the following relationship [1]:

$$\frac{1}{2}(T_L - T_S)(c_{\max} + c_s) = c_m(T_L - T_S) + L \tag{13}$$

Distribution of c_{eff} can also be described using the curve of degree p (Fig. 2c) where p is usually accepted in the range of 5-7 [1]:

$$c_{eff}(T) = c_s + (p+1)\left(c_m + \frac{L}{T_L - T_S} - c_s\right)\left(\frac{T - T_S}{T_L - T_S}\right)^p \tag{14}$$

In addition to this one can find descriptions of c_{eff} based on the phase equilibrium diagram. Borisow (15) and Samojłowicz (16) models are examples of such an approach [1, 7]:

$$c_{eff}(T) = c_m + \frac{L}{(1-k)(T_p - T_z)}\left(\frac{T_p - T_z}{T_p - T}\right)^{\frac{2-k}{1-k}} \tag{15}$$

$$c_{eff}(T) = c_m - m_L m_S \frac{L(T_S - T_L)}{\left[m_L(T - T_L) - m_S(T - T_S)\right]^2} \tag{16}$$

where k is the coefficient of phase separation, T_p [K] - melting temperature of pure iron, T_z [K] - liquidus temperature at a given concentration z_0, m_L [-] - the slope of the liquidus line, m_S [-] - the slope of the solidus line.

2. Numerical scheme

Starting from the criterion of the method of weighted residuals [8] equation (6) is multiplied by the weighting function w and integrated over the region $\Omega = \Omega_S \cup \Omega_L \cup \Omega_{S+L}$:

$$\int_{\Omega} w\left[\frac{\partial}{\partial x}\left(\lambda_m \frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda_m \frac{\partial T}{\partial y}\right)-\rho_m c_{eff}\frac{\partial T}{\partial t}\right]d\Omega = 0 \tag{17}$$

Further the weak form of (6) can be written as the following sum of integral terms

$$\int_{\Omega}\lambda_m\left(\frac{\partial w}{\partial x}\frac{\partial T}{\partial x}+\frac{\partial w}{\partial y}\frac{\partial T}{\partial y}\right)d\Omega+\int_{\Omega} w\rho_m c_{eff}\frac{\partial T}{\partial t}d\Omega = -\int_{\Gamma} w q_b d\Gamma \tag{18}$$

where q_b is heat flux normal to the external boundary Γ.

Using Galerkin formulation [8] $w_i(x, y) = N_i(x,y)$ is adopted, where N_i are the shape functions of the finite element. This assumption leads to the local energy equation in the following form:

$$\lambda_m^{(e)}\int_{\Omega^{(e)}}\left(\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x}+\frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y}\right)d\Omega T_j+\left(\rho_m c_{eff}\right)^{(e)}\int_{\Omega^{(e)}} N_i N_j d\Omega\frac{\partial T_j}{\partial t} = -\int_{\Gamma^{(e)}} N_i q_b d\Gamma \tag{19}$$

Integral terms appearing in equation (19) can be replaced by the corresponding elements of the following matrices:

$$K_{ij}^{(e)} = \lambda_m^{(e)}\int_{\Omega^{(e)}}\left(\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x}+\frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y}\right)d\Omega \tag{20}$$

$$M_{ij}^{(e)} = \left(\rho_m c_{eff}\right)^{(e)}\int_{\Omega^{(e)}} N_i N_j d\Omega \tag{21}$$

$$B_i^{(e)} = -\int_{\Gamma^{(e)}} N_i q_b d\Gamma \tag{22}$$

where $\mathbf{K}^{(e)}$ is local heat conductivity matrix, $\mathbf{M}^{(e)}$ - heat capacity matrix, $\mathbf{B}^{(e)}$ - right-hand side vector.

Using equations (20)-(22) the local FEM equation is written in the following form:

$$\mathbf{K}^{(e)}\mathbf{T}+\mathbf{M}^{(e)}\dot{\mathbf{T}} = \mathbf{B}^{(e)} \tag{23}$$

Derivative of the temperature with respect to time is approximated by the scheme shown below

$$\dot{\mathbf{T}} = \frac{\mathbf{T}^{f+1} - \mathbf{T}^{f}}{\Delta t}, \Delta t = t^{f+1} - t^{f} \tag{24}$$

where f is the level of time, Δt [s] - time step.

Using above scheme in equation (23) and aggregating over entire mesh the global equation is obtained

$$\left(\mathbf{K} + \frac{1}{\Delta t}\mathbf{M} \right) \mathbf{T}^{f+1} = \mathbf{B} + \frac{1}{\Delta t}\mathbf{M}\mathbf{T}^{f} \tag{25}$$

This equation results from the Euler's backward time discretization scheme [8].

Conclusions

The presented mathematical and numerical models of the binary alloy solidification process are the basis for creating a solver which makes it possible to out numerical simulations of solidification of steel.

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