JAM CM Journal of Applied Mathematics and Computational Mechanics 2015, 14(3), 121-126
www.amcm.pcz.pl p-ISSN 2299-9965
DOI: 10.17512/jamcm.2015.3.13 e-ISSN 2353-0588

NUMERICAL MODELING OF PURE METAL SOLIDIFICATION USING THE ONE DOMAIN APPROACH

Romuald Szopa

Faculty of Civil Engineering, Czestochowa University of Technology
Częstochowa, Poland
rszopa@word.katowice pl

Abstract. Numerical modeling of pure metal solidification on the basis of the well-known Stefan model is rather difficult. The knowledge of temporary solidification front position and the local values of the solidification rate in the normal direction for time t are necessary in order to determine the new position of moving boundary for time $t + \Delta t$. The problem is especially complicated for 2D and 3D tasks. The concept greatly simplifying the modeling of solidification process boils down to the introduction of the artificial region corresponding to the mushy zone sub-domain. For this region the substitute thermal capacity is defined and the mathematical model corresponds to the one domain approach. The artificial mushy zone appears owing to conventional enlargement of solidification point on a certain interval of temperature ΔT. The basic goal of the paper is the numerical analysis of the influence of the interval ΔT on the numerical solution simulating the thermal processes in the domain of the solidifying metal.

Keywords: *solidification of metals, Stefan problem, artificial mushy zone, numerical methods*

1. Introduction

Modeling of pure metals (more generally pure substances) solidification or melting called the Stefan problem [1] is a task frequently discussed in the literature. The characteristic feature of this type of tasks is the boundary condition given on the moving boundary between solid and liquid sub-domains. The numerical procedures simulating the movement of the moving boundary are rather complex, especially in the case of 2D or 3D problems (e.g. [2]). When the knowledge of an exact temporary shape of the moving boundary is not required and the sufficient information is the location of the front with accuracy to the element resulting from domain discretization then the relatively simple numerical procedures can be used. In this place the temperature recovery method [3-5] and the alternating phase truncation method [5-7] should be mentioned. The first one was proposed years ago by Ruddle and, generally speaking, its essence consists in the tracking of physical

enthalpy changes. During the time of the latent heat evolution the nodal temperature is kept at the constant level corresponding to the solidification point. The second one consists of the double solution of a heat diffusion problem for conventionally homogeneous metal domain (liquid and solid) and the appropriate correction of obtained temporary solutions.

Another approach to solve the Stefan problem is to use the mathematical model concerning the alloys solidification. The transition from a liquid to a solid state in the case of typical binary alloys proceeds in the interval of temperature. Between the border temperatures T_S and T_L the latent heat L is exhaled, while the domain limited by T_S and T_L is called a mushy zone.

The introduction of an artificial mushy zone requires the 'extension' of solidification point T^* on a certain interval of temperatures $[T^* - \Delta T,\ T^* + \Delta T]$. Next for this interval the substitute thermal capacity should be defined (see the next section). Finally, the Stefan problem is substituted by the mathematical model called in literature the one domain method [8, 9]. The aim of research presented in this paper is the analysis of a solidification problem solution obtained for different values of ΔT.

2. One domain method

Let us consider the following energy equation

$$c(T)\frac{\partial T(x,t)}{\partial t} = \nabla\left[\lambda(T)\nabla T(x,t)\right] + L\frac{\partial f_S(x,t)}{\partial t} \tag{1}$$

where $c(T)$ is a volumetric specific heat of metal, $\lambda(T)$ is a thermal conductivity, L is a volumetric latent heat, $T = T(x,\ t)$, $f_S = f_S(x,\ t)$ are the temperature and the local volumetric fraction of solid state, $x,\ t$ are the spatial co-ordinates and time.

To adapt equation (1) to numerical modeling of pure metals solidification, the sub-domain of artificial mushy zone must be introduced and we assume that it corresponds to the interval $[T^* - \Delta T,\ T^* + \Delta T]$. The energy equation corresponding to the one domain approach results from the assumption that the temperature-dependent function $f_S(T)$ in the interval $[T_S, T_L]$ is known, for example

$$f_S(T) = \frac{T^* + \Delta T - T(x,t)}{2\Delta T} \tag{2}$$

Because

$$\frac{\partial f_S(x,\ t)}{\partial t} = \frac{\mathrm{d} f_S(T)}{\mathrm{d} T}\ \frac{\partial T(x,\ t)}{\partial t} \tag{3}$$

therefore for the established form of function f_S one obtains

$$L\frac{\partial f_S(x,t)}{\partial t} = -\frac{L}{2\Delta T}\frac{\partial T(x,t)}{\partial t} \tag{4}$$

and finally

$$C(T)\frac{\partial T(x,t)}{\partial t} = \nabla\left[\lambda(T)\nabla T(x,t)\right] \tag{5}$$

where the parameter

$$C(T) = c(T) + \frac{L}{2\Delta T} = c_M + \frac{L}{2\Delta T} \tag{6}$$

is called a substitute thermal capacity of a mushy zone sub-domain. Summing up, the following definition of substitute thermal capacity can be accepted

$$C(T) = \begin{cases} c_L & T > T^* + \Delta T \\ c_M + \dfrac{L}{2\Delta T} & T^* - \Delta T \le T \le T^* + \Delta T \\ c_S & T < T^* - \Delta T \end{cases} \tag{7}$$

where c_L, c_M, c_S are the volumetric specific heats of molten metal, mushy zone and solid state sub-domains, wherein $c_M = (c_L + c_S)/2$. One can see that equation (5) can be used as the model of thermal processes proceeding in the whole, conventionally homogeneous, metal domain.

In Figure 1, the real course of enthalpy function for pure metal is shown. A diagonal line between the points $T^* - \Delta T$, $T^* + \Delta T$ illustrates the modified enthalpy function, while the substitute thermal capacity corresponds to the slopes of successive segments.

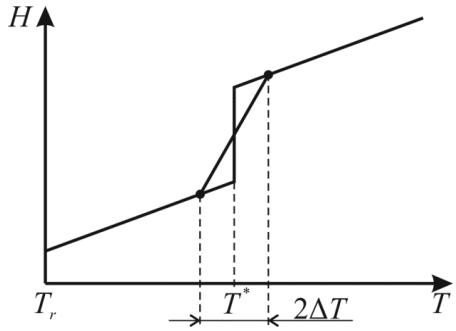

Fig. 1. Enthalpy function

The course of thermal conductivity is approximated by the broken line (the constant values for solid and liquid states and the segment joining the points $(T^* - \Delta T, \lambda_S)$ and $(T^* + \Delta T, \lambda_L)$.

3. Mathematical model of solidification process

The following boundary-initial problem is considered.

Non-steady temperature field in the metal domain is described by non-linear Fourier equation

$$C(T)\frac{\partial T(r,z,t)}{\partial t} = \nabla\left[\lambda(T)\nabla T(r,z,t)\right] \tag{8}$$

where r, z denote the cylindrical co-ordinates (an axially-symmetrical task is considered - see next chapter), while the form of operator $\nabla\left[\lambda(T)\nabla T(r,z,t)\right]$ can be found, among others, in [5]. Equation (8) is supplemented by the similar equation determining the course of thermal processes in a mould sub-domain

$$c_m(T)\frac{\partial T_m(r,z,t)}{\partial t} = \nabla\left[\lambda_m(T)\,\nabla T_m(r,z,t)\right] \tag{9}$$

where c_m and λ_m denote the mould volumetric specific heat and mould thermal conductivity.

On the external surface of the mould the boundary condition in a general form

$$\Phi\left[T_m(r,z,t), \frac{\partial T_m(r,z,t)}{\partial n}\right] = 0 \tag{10}$$

is accepted, whereas $\partial/\partial n$ denotes a normal derivative.

On the contact surface between the casting and mould the continuity condition is given

$$-\lambda\frac{\partial T(r,z,t)}{\partial n} = \frac{T(r,z,t) - T_m(r,z,t)}{R(r,z,t)} = -\lambda_m\frac{\partial T_m(r,z,t)}{\partial n} \tag{11}$$

where R is a thermal resistance. For $R = 0$ (at the stage of numerical computations such an assumption has been done) the last condition takes a form

$$\begin{cases} -\lambda\dfrac{\partial T(r,z,t)}{\partial n} = -\lambda_m\dfrac{\partial T_m(r,z,t)}{\partial n} \\ T(r,z,t) = T_m(r,z,t) \end{cases} \tag{12}$$

The initial temperature for $t = 0$ is also known

$$T(r, z, 0) = T_0, \qquad T_m(r, z, 0) = T_{m0} \tag{13}$$

The numerical solution of the problem discussed has been found using the explicit scheme of finite difference method in the version in detail presented in [5].

4. Examples of computations

The aluminum bar produced in the typical sand mix mould is considered. The casting dimensions are equal to $R = 2$ cm, $H = 8$ cm. Thermophysical parameters of materials: $c_S = 2.7$ MJ/m^{3}K, $c_L = 3.07$ MJ/m^{3}K, $c_M = 2.885$ MJ/m^{3}K, $L = 1053$ MJ/m^3, $\lambda_S = 240$ W/m K, $\lambda_L = 104$ W/m K, $T^* = 660$°C, $c_m = 1.75$ MJ/m^3, $\lambda_m = 1$ W/m K. The initial temperature of the metal domain equals 700°C, while the initial temperature of the mould equals 30°C. The successive simulations have been done for $\Delta T = 3, 5, 7$ K. In Figure 2 the cooling curves at the central point of casting ($r = 0$, $z = 4$ cm) are shown. The numbers 1, 2, 3 correspond to $\Delta T = 3, 5, 7$ K.

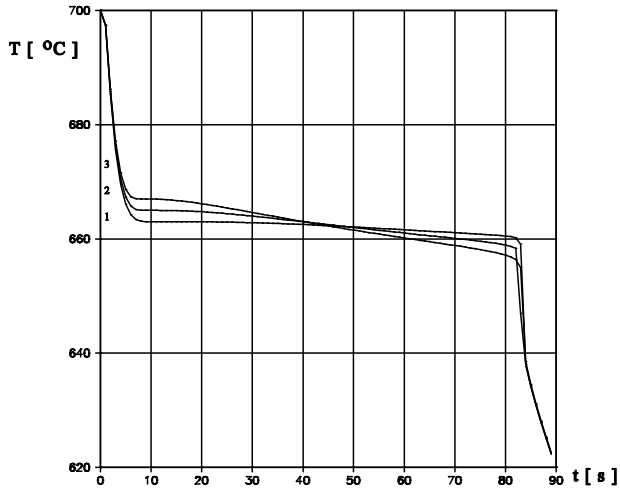

Fig. 2. Cooling curves

5. Conclusions

One can see that the results of numerical simulation are similar and the value of ΔT is not very essential. This information can be important for the researchers working in the field of numerical modeling of solidification, because the concept presented is quite simple and effective at the stage of numerical computations. Because the changes of substitute thermal capacity at the crossing by the border isotherms are considerable, one should supplement the basic algorithm by the

introduction of correcting procedures presented in [4, 5]. Additionally, taking into account the small temperature interval corresponding to the artificial mushy zone sub-domain, the time step assumed should be small (for example 10% of time step resulting from the stability condition of the explicit scheme of the finite difference method).

References

[1] Vulk C., Some historical notes about the Stefan problem, Nieuw Archief voor Wiskunde 1993, 4e serie 11 (2), 157-167.

[2] Nowak I., Smolka J., Nowak A., A reproduction of boundary conditions in three-dimensional continuous casting problem, International Journal of Mathematical, Physical and Engineering Sciences 2009, 3-4, 193-198.

[3] Ruddle R.W., The Solidification of Casting, The Institute of Metals, London 1957.

[4] Szopa R., Modeling of Solidification and Crystallization Using the Combined Variant of the BEM, Metallurgy 54, Publication of the Silesian University of Technology, Gliwice 1999 (in Polish).

[5] Mochnacki B., Suchy J.S., Numerical Methods in Computations of Foundry Processes, PFTA, Cracow 1996.

[6] Majchrzak E., Mochnacki B., Application of the BEM in the thermal theory of foundry, Engineering Analysis with Boundary Elements 1995, 16, 2, 99-121.

[7] Slota D., Homotopy perturbation method for solving the two-phase inverse Stefan problem, Numer. Heat Transfer A 2011, 59, 755-768.

[8] Majchrzak E., Mochnacki B., Suchy J.S., Identification of substitute thermal capacity of solidifying alloy, Journal of Theoretical and Applied Mechanics 2008, 46, 2, 257-268.

[9] Mochnacki B., Szopa R., Numerical modeling of solidification. Substitute thermal capacity of binary alloy, Advanced Diffusion Processes and Phenomena, Book Series: Defect and Diffusion Forum, 2014, 354, 33-40.