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Model of pure metal solidification using the power-type function

B. Mochnacki*, R. Szopa
Institute of Mathematics and Computer Science, Czestochowa University of Technology, ul. Dąbrowskiego 73, 42-200, Czestochowa, Poland
* Corresponding author: E-mail address: moch@imi.pcz.pl

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Analysis and modelling

ABSTRACT

Purpose: The typical mathematical descriptions of pure metal solidification (micro/macro approach) base on the linear or exponential (Kolmogoroff) models. In the paper the possibilities of such models modification are presented. This new model can be called a power type one. The approach proposed can be useful on the stage of numerical simulation of solidification on the micro/macro scale.
Design/methodology/approach: The local and temporary volumetric fraction of solid state is described by the equation from which both the linear and exponential model can be obtained. Introducing the additional parameter to this equation the new solidification model is found.
Findings: The method here presented allows to determine the transient temperature field in a non-homogeneous system casting-mould and to observe the course of metal solidification. The obtained cooling curves allow to observe (contrary to macro models) the recalescence effect.
Practical implications: The solidification model in a version presented in this paper can be an effective tool for numerical simulation of solidification process.
Originality/value: The concept of introduction of power-type function for the mathematical description of micro/macro solidification model is original and gives the new possibilities numerical methods application in a thermal theory of foundry processes.
Keywords: Numerical techniques; Solidification of metals; Micro/macro models

1. Introduction

The heat transfer processes proceeding in the solidifying casting volume (only heat conduction is taken into account) are described by the following energy equation [1-4, 15]

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

where $c(T)$ is a volumetric specific heat, $\lambda(T)$ is a thermal conductivity, q_V is a source function controlling the solidification process, T, x, t denote the temperature, spatial co-ordinates and time. The last component in equation (1) equals

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

where L is a volumetric latent heat, f_S is a volumetric solid state fraction at the point considered.

On the outer surface of the system the condition in general form

$$\Phi\left[T(x,t),\ \frac{\partial T(x,t)}{\partial n}\right]=0 \tag{3}$$

is given, where $\partial/\partial n$ denotes a normal derivative.

The initial condition

$$t = 0: \qquad T(x, 0) = T_0 \tag{4}$$

is also known.

More complex and close to the real situation mathematical models take into account the presence of the mould sub-domain. Then the equation (1) is supplemented by the equation

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

where c_M is a mould volumetric specific heat, λ_M is a mould thermal conductivity. In the case of typical sand molds on the contact surface between casting and mould the continuity condition in the form

$$\begin{cases} -\lambda\dfrac{\partial T(x,t)}{\partial n} = -\lambda_M\dfrac{\partial T_M(x,t)}{\partial n} \\ T(x,t) = T_M(x,t) \end{cases} \tag{6}$$

can be accepted. Additionally on the external surface of the mould we have

$$-\lambda_M\frac{\partial T_M(x,t)}{\partial n} = \alpha\left[T_M(x,t) - T_a\right] \tag{7}$$

where α is a heat transfer coefficient, T_a is an ambient temperature. The initial mould temperature is also given. From the numerical point of view the algorithm in which the thermal processes in the mould sub-domain are taken into account is more time-consuming, but similar to the simpler one.

The micro/macro models of solidification (the second generation ones) basing on the assumption that the kinetic of nucleation and nuclei growth are proportional to the undercooling below the solidification point are discussed. In particular, the linear model described among others in [5,6,7], the exponential one [8-11] and its modification [8,12-15] are considered. The aim of our research is to modify the mentioned above approaches and to introduce the power-type function model.

2. Micro/macro models of solidification

In the group of models here discussed we introduce the following function

$$\omega(x,t) = N(x,t)\ V(x,t) \tag{8}$$

where N is a grains density [grains/m^3], V is a single grain volume. If we consider the spherical grains and $u = \partial R/\partial t$ is a crystallization rate (R is a grain radius) then

$$V(x,t) = \frac{4}{3}\pi\left[\int_0^t u(\tau)\,\mathrm{d}\tau\right]^3 \tag{9}$$

In the case of the others types of crystallization (e.g. dendritic growth) the coefficient $\nu < 1$ can be introduced [12] and then

$$V(x,t) = \frac{4}{3}\pi\nu\left[\int_0^t u(\tau)\,\mathrm{d}\tau\right]^3 \tag{10}$$

Finally

$$\omega(x,t) = \frac{4}{3}\pi\nu\int_0^t \frac{\partial N(x,t)}{\partial t}\left[\int_0^t u(\tau)\,\mathrm{d}\tau\right]^3 \mathrm{d}t \tag{11}$$

The numerical aspects of this function computations are discussed, among others, in [6, 7].

In the case of so-called linear model the function f_S is assumed to be equal $\omega(x,t)$:

$$f_S(x,t) = \omega(x,t) \tag{12}$$

and if $f_S = 1$ then the crystallization process stops. The derivative of f_S with respect to time equals

$$\frac{\partial f_S(x,t)}{\partial t} = \frac{\partial \omega(x,t)}{\partial t} \tag{13}$$

One can see that equation (11) determines the geometrical volume (volume fraction) and it is the correct assumption on the first stages of crystallization. In order to take into account the geometrical limitations of growth in the final stages of the process the equation (13) can be modified to the form [5]

$$\frac{\partial f_S(x,t)}{\partial t} = \frac{\partial \omega(x,t)}{\partial t}\left[1 - f_S(x,t)\right] \tag{14}$$

It can be shown that the exponential model resulting from the theory proposed by Mehl, Johnson, Avrami and Kolmogoroff can be also found directly using the last equation. So, we transform the equation (14) to the following form

$$\frac{\mathrm{d}f_S(\omega)}{1 - f_S(\omega)} = \mathrm{d}\omega \tag{15}$$

and next

$$f_S(\omega) = 1 + C\exp(-\omega) \tag{16}$$

Because for $\omega = 0$: $f_S = 0$ therefore $C = -1$ and finally

$$f_S(\omega) = 1 - \exp(-\omega) \tag{17}$$

The equation (17) corresponds to the well known Kolmogoroff formula. One can see that for the small geometrical volumes $\exp(-\omega) = 1 - \omega$ and the equations (12), (17) lead to the same results.

The formula (14) can be modified to the other form, namely

$$\frac{\partial f_S(x,t)}{\partial t} = \frac{\partial \omega(x,t)}{\partial t}\left[1 - f_S(x,t)\right]^n \tag{18}$$

where $n \geq 0$. From the physical point of view the same conditions as in case of (14) are fulfilled and the component $1 - f_S$ changes from 0 to 1, while the generalized form of (15) is then the following

$$\frac{\mathrm{d} f_S(\omega)}{\left[1 - f_S(\omega)\right]^n} = \mathrm{d}\omega \tag{19}$$

The solution fulfilling the condition $\omega = 0$: $f_S = 0$ is of the form

$$f_S(\omega) = 1 - \left[(n-1)\omega + 1\right]^{\frac{1}{1-n}} \tag{20}$$

One can see that the last power-type formula constitutes the generalization of linear and exponential models. For $n = 0$ one obtains the equation (12), while for $n = 1$ one has

$$\lim_{n \to 1}\left\{1 - \left[(n-1)\omega + 1\right]^{\frac{1}{1-n}}\right\} = 1 - \exp(-\omega) \tag{21}$$

which correspond to (17). The others values of n can be also be taken into account. For example

$$\begin{aligned} n = 2: &\qquad f_S = 1 - \frac{1}{\omega + 1} \\ n = 3: &\qquad f_S = 1 - \frac{1}{\sqrt{2\omega + 1}} \\ n = \frac{1}{2}: &\qquad f_S = 1 - \left(1 - \frac{\omega}{2}\right)^2 \end{aligned} \tag{22}$$

It should be pointed out that if $n \geq 1$ then for $\omega \to \infty$: $f_S \to 1$. This property is not fulfilled for $n < 1$ and it must be taken into account on the stage of numerical simulation. For example if $n = 1/2$ then solidification process takes place only for $\omega \geq 2$, the values $\omega > 2$ are not physically correct.

Additionally considering the group of models discussed it is assumed that a local and temporary number of nuclei is proportional to the second power of undercooling below the solidification point T^*

$$N(x,t) = \eta \Delta T(x,t)^2 = \eta\left[T^* - T(x,t)\right]^2 \tag{23}$$

where η is the nucleation coefficient. The nucleations stops when

$\Delta T(x, t + \Delta t) < \Delta T(x,t)$, for $T(x,t) > T^* \quad N(x,t) = 0$.

The nuclei growth is determined by the formula

$$\frac{\mathrm{d} R(x,t)}{\mathrm{d} t} = \mu \Delta T^m(x,t) \tag{24}$$

where μ is the growth coefficient, $m \in [1,\ 2]$ (see: [12,14]). One can find also the other equation, namely

$$u(x,t) = \frac{\mathrm{d} R(x,t)}{\mathrm{d} t} = \mu_1 \Delta T(x,t)^2 + \mu_2 \Delta T(x,t)^3 \tag{25}$$

where μ_1, μ_2 are the growth coefficients.

The details concerning the numerical aspects of solidification process modelling will be not here discussed. The information from this scope can be found, among others in [2, 3, 8].

3. Example of computations

The aluminium plate ($G/2 = 0.01$ m) produced in typical sand mould has been considered. The input data concerning the materials can be found in [1]. The method of source function modelling is discussed in [3].

In Figure 1 the cooling curves at the point located close to the casting-mould contact surface are shown. They correspond to parameters $n = 1$ (Kolmogoroff model) and $n = 2$ (power-type model). The differences between the results obtained are not big, but visible. The authors are not able to answer which ones are better. It requires the exact verification with the experiments. In spite of this, it should be pointed out that both results correspond to the real courses of typical cooling curves and the power-type model most certainly constitutes an effective generalization of the models described in literature.

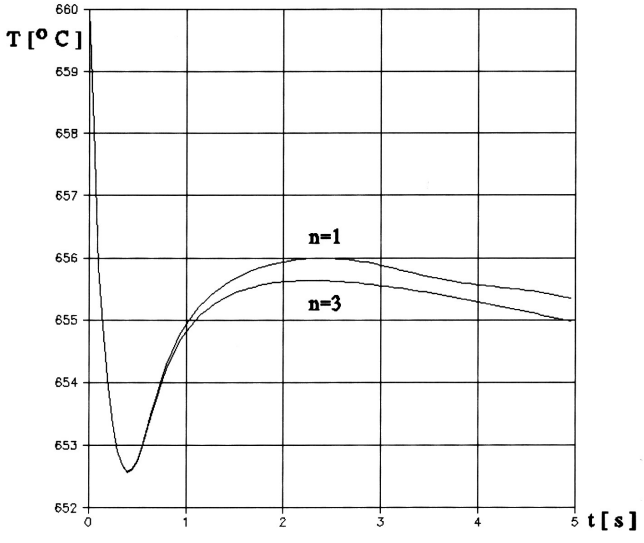

Fig. 1. Cooling curves

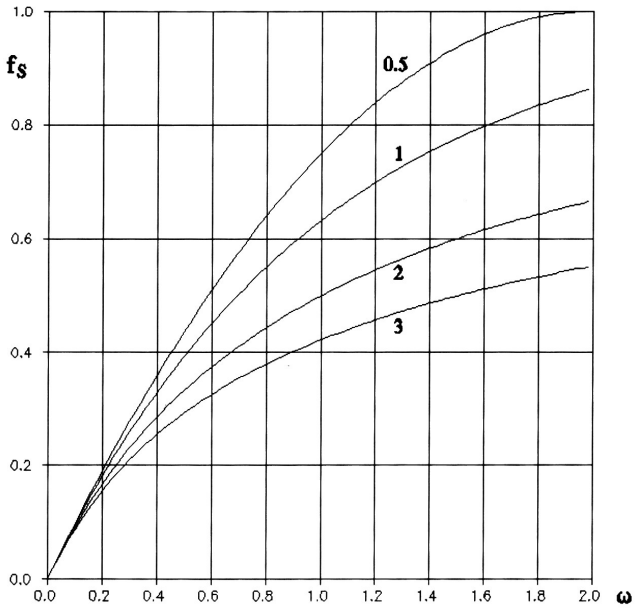

Fig. 2. Functions $f_S(\omega)$

In Figure 2 the functions $f_S(\omega)$ for different values of ω are shown. One can see that in the case of big nuclei density (close-grained structure) the value of n is fractional, while in the case of small nuclei density (coarse-grained structure) the value of n should be assumed more than 1. The possibility of local values of n introduction can be also taken into account.

4. Conclusions

The generalization of well known Mehl-Johnson-Avrami-Kolmogoroff approach gives the possibilities of new solidification models construction . They models can be useful on the stage of numerical simulation of thermal processes proceeding in the casting-mould system.

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