LINEAR AND EXPONENTIAL MODELS
OF CRYSTALLIZATION PROCESS SIMULATION

Bohdan Mochnacki, Edyta Pawlak

Institute of Mathematics and Computer Science, Czestochowa University of Technology

Abstract. In the paper the micro/macro models of crystallization are considered. In literature they are called also the second generation ones. The approach considered bases on the nucleation and nuclei growth laws. The 'driving force' of these phenomena is the undercooling below the solidification point. In particular, the linear model described among others in [1], the exponential one [2, 3] and its modification [4, 5] are discussed. The aim of research presented is the estimation of assumed model influence on the results of numerical simulation of crystallization process. The numerical algorithm bases on the finite differences method. In the final part of the paper the numerical example is presented.

1. Mathematical description of the process

The following energy equation concerning the casting domain is considered [6]

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

where c is a volumetric specific heat, λ is a thermal conductivity, L is a volumetric latent heat, f_S is a volumetric solid state fraction at the considered point from casting domain, T, x, t denote the temperature, geometrical co-ordinates and time.
Equation (1) can be used both in the case of macro models [6, 7] (then the substitute thermal capacity is, as a rule, introduced) and in the case of micro/macro models [2-5] (this case is considered in the paper).

The similar equation determines the temperature field in the mould sub-domain namely

$$c_M(T)\frac{\partial T_M(x,t)}{\partial t} = \nabla\left[\lambda_M(T)\nabla T_M(x,t)\right] \qquad (2)$$

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

$$\begin{cases} -\lambda \dfrac{\partial T(x,t)}{\partial n} = -\lambda_M \dfrac{\partial T_M(x,t)}{\partial n} \\[2mm] T(x,t) = T_M(x,t) \end{cases} \tag{3}$$

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

$$-\lambda_M \frac{\partial T_M(x,t)}{\partial n} = \alpha \left[T_M(x,t) - T_a \right] \tag{4}$$

where α is a heat transfer coefficient, T_α is an ambient temperature.
The initial condition

$$t = 0 \; : \;\; T(x,0) = T_0 \, , \; T_M(x,0) = T_{M0} \tag{5}$$

is also known.

2. Models of crystallization

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

$$\omega(x,\,t) = N(x,\,t)\,v(x,\,t) \tag{6}$$

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

$$v(x,t) = \frac{4}{3}\pi \left[\int_0^t u(\tau)\,\mathrm{d}\tau \right]^3 \tag{7}$$

In the case of the others types of crystallization (e.g. dendritic growth) the coefficient $v < 1$ can be introduced [4] and then

$$v(x,t) = \frac{4}{3}\pi v \left[\int_0^t u(\tau)\,\mathrm{d}\tau \right]^3 \tag{8}$$

Finally

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

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

$$f_s(x,t) = N(x,\,t)\,v(x,\,t) \tag{10}$$

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

$$\frac{\partial f_s(x,t)}{\partial t} = 4\pi v \left[\frac{R^3(x,t)}{3} \frac{\partial N(x,t)}{\partial t} + R^2(x,t) \frac{\partial R(x,t)}{\partial t} N(x,t) \right] \tag{11}$$

One can see that equation (10) 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 spherical growth in the final stages of the process the equation (11) is also modified to the form [1]

$$\frac{\partial f_s}{\partial t} = 4\pi v \left[\frac{R^3}{3} \frac{\partial N}{\partial t} + R^2 \frac{\partial R}{\partial t} N \right] (1 - f_s) \tag{12}$$

The exponential model resulting from the theory proposed by Mehl, Johnson, Avrami and Kolmogoroff (e.g. [2, 3]) bases on the following formula

$$f_s(x,t) = 1 - \exp\left[-\omega(x,t)\right] = 1 - \exp\left\{ -\frac{4}{3}\pi v\, N(x,t) \left[\int_0^t u(\tau)\,\mathrm{d}\tau \right]^3 \right\} \tag{13}$$

in other words the expression of type (6) corresponds to the exponent in equation (13). For the small geometrical volumes $\exp(-\omega) = 1 - \omega$ and the formulas (10), (13) are the same.
Additionally considering the group of models discussed it is assumed that:
1) A local and temporary number of nuclei is proportional to the second power of undercooling below the solidification point T^*

$$N(x,t) = \eta\,\Delta T^2(x,t) = \eta \left[T^* - T(x,t) \right]^2 \tag{14}$$

where η is the nucleation coefficient.
The nucleations stops when $\Delta T(x, t + \Delta t) < \Delta T(x,t)$, for $T(x,t) > T^*$ $N(x,t) = 0$.
2) The nuclei growth is determined by the formula

$$\frac{\mathrm{d}R(x,t)}{\mathrm{d}t} = \mu\,\Delta T^m(x,t) \tag{15}$$

where μ is the growth coefficient, $m \in [1,2]$ (see [2, 3]).

One can find also the other equation, namely

$$u(x,t) = \frac{d\,R(x,t)}{d\,t} = \mu_1\,\Delta T^2(x,t) + \mu_2\,\Delta T^3(x,t) \tag{16}$$

where μ_1, μ_2 are the growth coefficients.

The interesting modification of Mehl - Johnson - Avrami - Kolmogoroff approach can be found in [4, 5].

In numerical realization the temporary value of exponent ω results from the following considerations [5].

At first the time grid is introduced

$$0 = t^0 < t^1 < t^2 < ... < t^f < t^{f+1} < ... < t^F, \quad \Delta t = t^{f+1} - t^f \tag{17}$$

while the casting domain is divided into control volumes V_i, $i = 1,2,3,..., n$.

So in order to determine the exponent ω for time t^{f+1} the successive 'portions' of solidifying metal should be registered

$$\omega(x_i, t^{f+1}) = \delta V_i^{\,1} + \delta V_i^{\,2} + ... + \delta V_i^{\,f} + \delta V_i^{\,f+1} \tag{18}$$

So

$$\begin{aligned}
f_L(x_i, t^{f+1}) &= \exp\left[-\omega(x_i, t^{f+1})\right] = \\
&= \exp\left[-\left(\delta V_i^{\,1} + \delta V_i^{\,2} + ... + \delta V_i^{\,f} + \delta V_i^{\,f+1}\right)\right] = \\
&= \exp\left(-\delta V_i^{\,1}\right) \cdot \exp\left(-\delta V_i^{\,2}\right) \cdot ... \cdot \exp\left(-\delta V_i^{\,f}\right) \cdot \exp\left(-\delta V_i^{\,f+1}\right)
\end{aligned} \tag{19}$$

where $f_L = 1 - f_S$ (a liquid state fraction).

Taking into account the small increments of $\delta V_i^{\,f}$ we can used the simple form of Taylor formula and then

$$f_L(x_i, t^{f+1}) = \left(1 - \delta V_i^{\,1}\right) \cdot \left(1 - \delta V_i^{\,2}\right) \cdot ... \cdot \left(1 - \delta V_i^{\,f+1}\right) \tag{20}$$

A certain modification of exponent ω definition is presented in [8].

The molten metal control volume V_i is considered.

Let us assume that during the transition from t^0 to t^1 the part $\delta V_i^{\,f}$ of V_i changes the phase.

At time t^1 the volume of liquid phase equals

$$V_i^1 = V_i - \delta V_i^1 = V_i\left(1 - \frac{\delta V_i^1}{V_i}\right) = V_i\left(1 - \hat{\delta} V_i^1\right) \tag{21}$$

where

$$\hat{\delta} V_i^1 = \frac{\delta V_i^1}{V_i} \tag{22}$$

In the second time interval the phase change can take place only in the volume V_i^1

$$V_i^2 = V_i^1 - \delta V_i^2 = V_i^1 \left(1 - \frac{\delta V_i^2}{V_i^1} \right) \tag{23}$$

or

$$V_i^2 = V_i \left(1 - \hat{\delta} V_i^1 \right)\left(1 - \hat{\delta} V_i^2 \right) \tag{24}$$

Analogously for time t^{f+1} we have

$$V_i^{f+1} = V_i \left(1 - \hat{\delta} V_i^1 \right)\left(1 - \hat{\delta} V_i^2 \right) \dots \left(1 - \hat{\delta} V_i^{f+1} \right) \tag{25}$$

or dividing by V_i

$$f_L \left(x_i, t^{f+1} \right) = \left(1 - \hat{\delta} V_i^1 \right)\left(1 - \hat{\delta} V_i^2 \right) \dots \left(1 - \hat{\delta} V_i^{f+1} \right) \tag{26}$$

At the same time

$$\hat{\delta} V_i^{f+1} = \frac{\delta V_i^{f+1}}{V_i^f} \tag{27}$$

The differences between formulas (20) and (26) are visible, but it turned out that results of numerical simulations are close.

3. Example of computation

As the example the aluminium plate of thickness 2.5 cm made in typical sand mould is considered (Fig. 1).

The following thermophysical parameters have been assumed:

- volumetric specific heat of casting domain $c = 3$ MJ/m³K,
- thermal conductivity of casting domain $\lambda = 150$ W/mK,
- volumetric latent heat $L = 975$ MJ/m³,
- nuclei density $N = 5 \cdot 10^{10}$ nuclei/m³,
- growth coefficient $\mu = 0.000003$ m/sK,
- volumetric specific heat of mould domain $c_M = 1.6$ MJ/m³K,
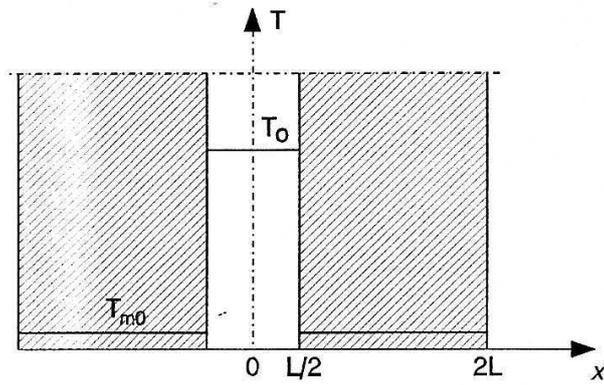- thermal conductivity of mould domain $\lambda_M = 1.5$ W/mK.

Fig. 1. Casting - mould domain

On the stage of numerical computations the FDM has been used both in the case of the linear model and in the case of exponential one. In Figures 2 and 3 the numerical solutions are shown. The numbers 1,2 correspond to the nodes close to the contact surface, number 4 corresponds to the casting axis, while number 3 to the central point of casting domain.

The numerical simulations shown that the results obtained using the linear model are close to the exponential one. So from numerical point of view it is a better to use the linear approach which is mathematically simpler than others models.
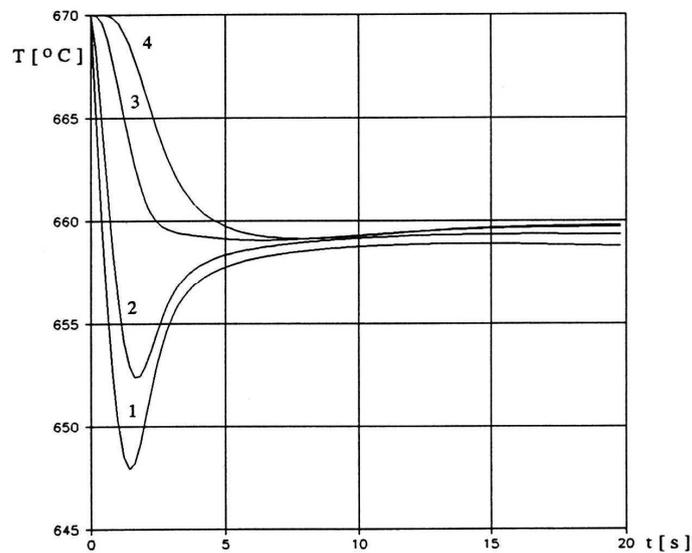

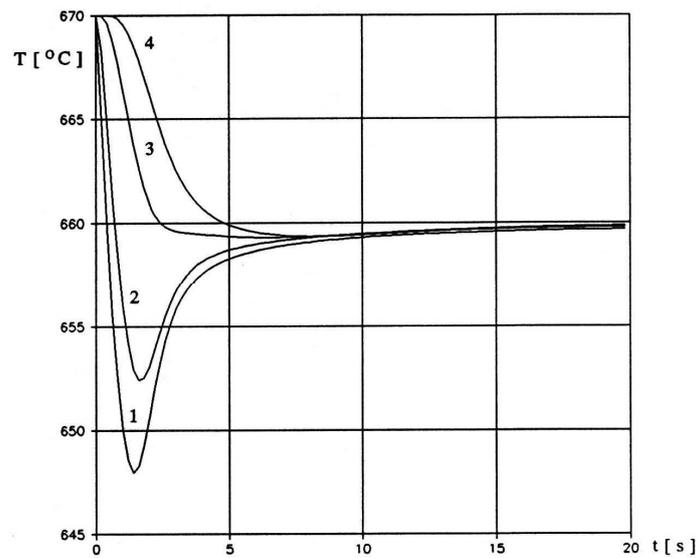Fig. 2. The results of exponential model application

Fig. 3. The results of linear model application

Acknowledgement

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