

Definition of Alloy Substitute Thermal Capacity Using the Simple Macrosegregation Models

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Abstract

Mathematical description of alloys solidification in a macro scale can be formulated using the one domain method (fixed domain approach). The energy equation corresponding to this model contains the parameter called a substitute thermal capacity (STC). The analytical form of STC results from the assumption concerning the course of the function $f_S = f_S(T)$ describing the changes of solid state volumetric fraction and the temperature at the point considered. Between border temperatures T_S, T_L the function f_S changes from 1 to 0. In this paper the volumetric fraction f_S (more precisely $f_L = 1 - f_S$) is found using the simple models of macrosegregation (the lever arm rule, the Scheil model). In this way one obtains the formulas determining the course of STC resulting from the certain physical considerations and this approach seems to be closer to the real course of thermal processes proceeding in domain of solidifying alloy.

Keywords: Application of Information Technology to the Foundry Industry, Solidification Process, One Domain Method, Substitute Thermal Capacity, Numerical Methods

1. One domain method

We consider the following energy equation

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

where $c(T)$ is a volumetric specific heat of casting material, $\lambda(T)$ is a thermal conductivity, L is a volumetric latent heat, $T = T(x, t)$, $f_S = f_S(x, t)$ denote the temperature and the local volumetric fraction of solid state. One can see, that only heat conduction in a casting volume is considered. The different forms of equation (1) appear at the stage of solidification rate $\partial f_S / \partial t$ computations (e.g. [1, 2]).

Let us denote the temperatures corresponding to the beginning and the end of solidification process by T_L and T_S , at the same time we assume the knowledge of temperature-dependent function f_S for the interval $[T_S, T_L]$ and then

$$\frac{\partial f_S(x, t)}{\partial t} = \frac{df_S}{dT} \frac{\partial T(x, t)}{\partial t} \quad (2)$$

Introducing this formula to energy equation (1) one obtains

$$C(T) \frac{\partial T(x,t)}{\partial t} = \nabla [\lambda(T) \nabla T(x,t)] \quad (3)$$

where $C(T) = c(T) - L df_S / dT$ is called 'a substitute thermal capacity'. This parameter can be defined in the different ways, it

will be discussed in the next part of the paper. One can see that for $T < T_S$: $f_S = 0$, while for $T > T_L$: $f_S = 1$ and the derivative $df_S/dT = 0$. Summing up, the following definition of substitute thermal capacity can be accepted [3, 4]

$$C(T) = \begin{cases} c_L & T > T_L \\ c_p - L \frac{df_S}{dT} & T_S \leq T \leq T_L \\ c_S & T < T_S \end{cases} \quad (4)$$

or, because $f_L = 1 - f_S$

$$C(T) = \begin{cases} c_L & T > T_L \\ c_p + L \frac{df_L}{dT} & T_S \leq T \leq T_L \\ c_S & T < T_S \end{cases} \quad (5)$$

where c_L , c_p , c_S are the volumetric specific heats of molten metal, mushy zone and solid state sub-domains and one can use the equation (3) as the model of thermal processes proceeding in the whole, conventionally homogeneous, casting domain. It is the reason that the approach presented is called 'a one domain method'. As an example of purely mathematical hypothesis concerning the course of function f_S , the formula

$$f_S(T) = \left(\frac{T_L - T}{T_L - T_S} \right)^n \quad (6)$$

can be considered. The function (6) fulfils the necessary condition $f_S(T_L) = 0$ and $f_S(T_S) = 1$, additionally it is the monotonic one. We find the derivative

$$\frac{df_S(T)}{dT} = -\frac{n}{T_L - T_S} \left(\frac{T_L - T}{T_L - T_S} \right)^{n-1} \quad (7)$$

and then

$$C(T) = c_p + \frac{L}{T_L - T_S} n \left(\frac{T_L - T}{T_L - T_S} \right)^{n-1} \quad (8)$$

The quotient $L / (T_L - T_S) = c_{sp}$ is called 'a spectral latent heat'. Introducing this parameter on has

$$C(T) = c_p + c_{sp} n \left(\frac{T_L - T}{T_L - T_S} \right)^{n-1} \quad (9)$$

Above formula is very often used for the case $n=1$, namely

$$C(T) = c_p + \frac{L}{T_L - T_S} = c_p + c_{sp}, \quad T \in [T_S, T_L] \quad (10)$$

The typical mathematical description of the real foundry technology requires the supplement of equation (1) by the equation determining the course of thermal processes in a mould sub-domain, this means

$$c_m(T) \frac{\partial T_m(x, t)}{\partial t} = \nabla \left[\lambda_m(T) \nabla T_m(x, t) \right] \quad (11)$$

where the index m identifies the mould sub-domain, the non-homogeneous mould can be also considered.

On the external surface of mould the following boundary condition

$$-\lambda_m \frac{\partial T_m(x, t)}{\partial n} = \alpha [T_m(x, t) - T_a] \quad (12)$$

is, as a rule, accepted. Here α is a heat transfer coefficient, T_a is an ambient temperature, $\partial/\partial n$ denotes a normal derivative.

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

$$-\lambda \frac{\partial T(x, t)}{\partial n} = \frac{T(x, t) - T_m(x, t)}{R(x, t)} = -\lambda_m \frac{\partial T_m(x, t)}{\partial n} \quad (13)$$

where R is a thermal resistance. For $R = 0$ (a such assumption can be done in the case of sand mix mould) the last equation takes a form

$$\begin{cases} -\lambda \frac{\partial T(x, t)}{\partial n} = -\lambda_m \frac{\partial T_m(x, t)}{\partial n} \\ T(x, t) = T_m(x, t) \end{cases} \quad (14)$$

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

$$t = 0: T(x, 0) = T_0(x), \quad T_m(x, 0) = T_{m0}(x) \quad (15)$$

The mathematical model presented above can be more complicated. For example, one can consider the convective component of heat transfer which appear in the molten metal sub-domain.

2. Macroseggregation models

Presented below the macroseggregation models result from the certain physical considerations concerning the mass (or volume) balance of alloy component in the casting volume. The models are close to the conditions of volumetric solidification. When the mass densities of liquid and solid are assumed to be the same, then the both balances lead to the same results. For two successive time levels t and $t+\Delta t$ we have the following form of volume balance

$$\begin{aligned} V_S(t) z_S(t) + V_L(t) z_L(t) = \\ V_S(t + \Delta t) z_S(t + \Delta t) + V_L(t + \Delta t) z_L(t + \Delta t) \end{aligned} \quad (16)$$

where z_S, z_L are the concentrations of alloy component in the solid and liquid phases. The change of volume $V_S(t + \Delta t) - V_S(t)$ is conventionally shown in Figure 1.

The values of V_S, V_L and z_S, z_L for time $t + \Delta t$ we can find using the Taylor series (the summands of higher order containing Δt^2 and next ones are neglected)

$$V_S(t + \Delta t) = V_S(t) + \frac{dV_S}{dt} \Delta t \quad (17)$$

$$V_L(t + \Delta t) = V_L(t) + \frac{dV_L}{dt} \Delta t \quad (18)$$

and similarly

$$z_S(t + \Delta t) = z_S(t) + \frac{dz_S}{dt} \Delta t \quad (19)$$

$$z_L(t + \Delta t) = z_L(t) + \frac{dz_L}{dt} \Delta t \quad (20)$$

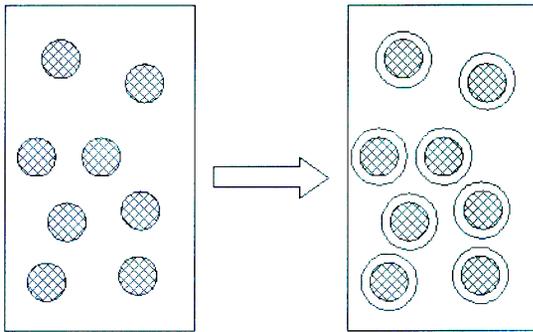


Fig. 1. The change of global $V_S(t)$

Using the equations (17) – (20) we obtain

$$V_S \frac{dz_S}{dt} + \frac{dV_S}{dt} z_S + V_L \frac{dz_L}{dt} + \frac{dV_L}{dt} z_L = 0 \quad (21)$$

or, taking into account the definitions of f_S and f_L

$$f_S \frac{dz_S}{dt} + \frac{df_S}{dt} z_S + f_L \frac{dz_L}{dt} + \frac{df_L}{dt} z_L = 0 \quad (22)$$

We introduce the partition coefficient $k = z_S / z_L$ and the self-evident dependence $f_S = 1 - f_L$ and then

$$(1 - f_L)k - \frac{df_L}{dz_L} k z_L + f_L + \frac{df_L}{dz_L} z_L = 0 \quad (23)$$

The final form of equation considered is the following

$$\frac{df_L}{dz_L} + \frac{f_L}{z_L} = -\frac{k}{1-k} \cdot \frac{1}{z_L} \quad (24)$$

The equation (24) is a linear one and it should be solved taking into account the condition $z = z_0 : f_L = 1$.

Let us assume that the partition coefficient is a constant value (it corresponds to the assumption that the lines T_S and T_L on the equilibrium diagram are the straight ones and they start from the same point T_p). The solution of equation (24) is of the form

$$f_L = \frac{z_0 - k z_L}{(1-k)z_L} \quad (25)$$

The last result correspond to the well known lever arm model.

We can also assume that the derivative $\frac{dz_S}{dt} = 0$ and then

$$\frac{df_S}{dt} z_S + f_L \frac{dz_L}{dt} + \frac{df_L}{dt} z_L = 0 \quad (26)$$

or

$$-\frac{df_L}{dz_L} k z_L + f_L + \frac{df_L}{dz_L} z_L = 0 \quad (27)$$

this means

$$\frac{df_L}{f_L} = -\frac{dz_L}{(1-k)z_L} \quad (28)$$

For $z = z_0 : f_L = 1$ and finally

$$f_L = \left(\frac{z_0}{z_L} \right)^{\frac{1}{1-k}} \quad (29)$$

The last equation corresponds to the Scheil model.

3. Substitute thermal capacity

Let us assume, as previously, that the partition coefficient k is a constant value. The straight lines determining the dependencies $T_S(z_S)$ and $T_L(z_L)$ are of the form

$$\begin{aligned} T_L &= T_p + a_L z_L \\ T_S &= T_p + a_S z_S \end{aligned} \quad (30)$$

and then

$$\begin{aligned} z_L &= \frac{T_L - T_p}{a_L} \\ z_0 &= \frac{T_0 - T_p}{a_L} \end{aligned} \quad (31)$$

where T_p is a solidification point of pure metal, T_0 is the border temperature corresponding to the concentration z_0 .

Because

$$\frac{df_L}{dT} = \frac{df_L}{dz_L} \frac{dz_L}{dT} = -\frac{z_0}{(1-k)z_L^2} \frac{1}{a_L} \quad (32)$$

consequently

$$C(T) = c_p - \frac{z_0}{(1-k)z_L^2} \frac{L}{a_L} \quad (33)$$

or introducing in a place of concentration the dependencies (31) we obtain

$$C(T) = c_p - \frac{L(T_0 - T_p)}{(1-k)(T - T_p)^2} \quad (34)$$

In the case of Scheil model one has

$$f_L = \left(\frac{T_0 - T_p}{T - T_p} \right)^{\frac{1}{1-k}} \quad (35)$$

and next

$$C(T) = c_p + \frac{L}{(1-k)(T_p - T_0)} \left(\frac{T_p - T_0}{T_p - T} \right)^{\frac{2-k}{1-k}} \quad (36)$$

One can see that for $T = T_0$ the liquid state fraction $f_L = 1$, while when the solidification process goes to the end f_L is not equal to 0. In this connection it should be assumed that the end of solidification corresponds, for example, to $f_L < 0.05$.

At the stage of numerical computations the following problem has been solved. The frame (2D problem – Figure 2) produced from Al-Si alloy (2% Si) has been considered. The following input data have been introduced: $c_S = 2.96 \text{ MJ/m}^3 \text{ K}$, $c_L = 3.07$, $\lambda_S = 250 \text{ W/mK}$, $\lambda_L = 104$, $L = 990.6 \text{ MJ/m}^3$, $k = 0.25$, $T_p = 660^\circ \text{C}$.

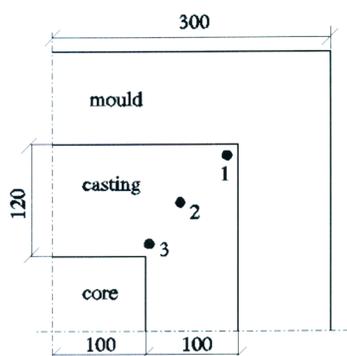


Fig. 2. Frame geometry

The remaining input data and the details concerning the numerical solution of a such problem can be found in the paper [5] developed by Szopa, Siedlecki and Wojciechowska from our team.

The example of results obtained concerns the application of equation (36). In particular, Figure 3 illustrates the cooling curves at the points 1, 2, 3 marked in Figure 2.

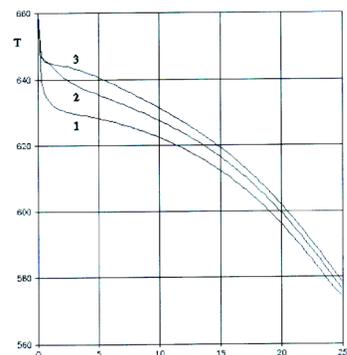


Fig. 3. Cooling curves

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