Definition of Alloy Substitute Thermal Capacity Using the Simple Macrosegregation Models

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Received 25.06.2012; accepted in revised form 03.09.2012

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

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

(1)

where \( \epsilon(T) \) 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 \( \frac{\partial f_S}{\partial t} \) 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

\[
\frac{\partial f_S(x,t)}{\partial t} = \frac{d f_S}{d T} \frac{\partial T(x,t)}{\partial t}
\]  

(2)

Introducing this formula into energy equation (1) one obtains

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

(3)

where \( C(T) = \epsilon(T) - L \frac{d f_S}{dT} \) 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 \( \frac{df_s}{dT} = 0 \).
Summing up, the following definition of substitute thermal capacity can be accepted [3, 4]

\[
C(T) = \begin{cases} 
  c_L & T > T_L \\
  c_p - L \frac{df_s}{dT} & T_s \leq T \leq T_L \\
  c_s & T < T_s
\end{cases} 
\]

(4)

or, because \( f_s = 1 - f_L \)

\[
C(T) = \begin{cases} 
  c_L & T > T_L \\
  c_p + L \frac{df_s}{dT} & T_s \leq T \leq T_L \\
  c_s & T < T_s
\end{cases} 
\]

(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

\[
f_s(T) = \left( \frac{T_L - T}{T_L - T_s} \right)^n
\]

(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

\[
\frac{df_s(T)}{dT} = -n \frac{T_s - T}{T_L - T_s} \left( \frac{T_L - T}{T_L - T_s} \right)^{n-1}
\]

(7)

and then

\[
C(T) = c_p + L \frac{df_s(T)}{dT} n \left( \frac{T_L - T}{T_L - T_s} \right)^{n-1}
\]

(8)

The quotient \( L / (T_L - T_s) = c_p \) is called ‘a spectral latent heat’. Introducing this parameter on has

\[
C(T) = c_p + c_p n \left( \frac{T_L - T}{T_L - T_s} \right)^{n-1}
\]

(9)

Above formula is very often used for the case \( n = 1 \), namely

\[
C(T) = c_p + \frac{L}{T_L - T_s} = c_p + c_p \cdot T \in [T_s, T_L]
\]

(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

\[
c_n(T) \frac{\partial T_n(x, t)}{\partial t} = \nabla \left[ \lambda_n(T) \nabla T_n(x, t) \right]
\]

(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

\[
-\lambda_n \frac{\partial T_n(x, t)}{\partial n} = \alpha [T_n(x, t) - T_a]
\]

(12)

is, as a rule, accepted. Here \( \alpha \) 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

\[
-\lambda_n \frac{\partial T_n(x, t)}{\partial n} = -\lambda_n \frac{\partial T_n(x, t)}{\partial n}
\]

(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

\[
\begin{cases} 
  -\lambda_n \frac{\partial T_n(x, t)}{\partial n} = -\lambda_n \frac{\partial T_n(x, t)}{\partial n} \\
  T(x, t) = T_n(x, t)
\end{cases}
\]

(14)

The initial temperature distribution for \( t = 0 \) is also known

\[
t = 0: \quad T(x, 0) = T_g(x), \quad T_n(x, 0) = T_{ng}(x)
\]

(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. Macrosegregation models

Presented below the macrosegregation 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

\[
V_s(t) z_s(t) + V_L(t) z_L(t) = V_s(t + \Delta t) z_s(t + \Delta t) + V_L(t + \Delta t) z_L(t + \Delta t)
\]

(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 \( \Delta t^2 \) and next ones are neglected)
Using the equations (17) – (20) we obtain

\[ V_s(t + \Delta t) = V_s(t) + \frac{dV_s}{dt} \Delta t \]  

\[ V_l(t + \Delta t) = V_l(t) + \frac{dV_l}{dt} \Delta t \]  

and similarly

\[ z_s(t + \Delta t) = z_s(t) + \frac{dz_s}{dt} \Delta t \]  

\[ z_l(t + \Delta t) = z_l(t) + \frac{dz_l}{dt} \Delta t \]  

\[ f_s = \frac{z_0 - k z_l}{(1-k) z_l} \]  

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

\[ \frac{df_s}{dz_l} z_s + f_l \frac{dz_l}{dt} + \frac{df_l}{dz_l} z_l = 0 \]  

or

\[ - \frac{df_s}{dz_l} k z_s + f_l + \frac{df_l}{dz_l} z_l = 0 \]  

this means

\[ \frac{df_s}{f_l} = - \frac{dz_s}{dz_l} \frac{1}{(1-k) z_l} \]  

For \( z = z_0 : f_s = 1 \) and finalny

\[ f_s = \left( \frac{z_0}{z_l} \right)^{\frac{1}{1-k}} \]  

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

\[ T_s = T_p + a_s z_s \]  

\[ T_l = T_p + a_l z_l \]  

and then

\[ z_s = \frac{T_s - T_p}{a_s} \]  

\[ z_l = \frac{T_l - T_p}{a_l} \]  

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

Because

\[ \frac{df_s}{df_l} = \frac{df_s}{dz_s} \frac{dz_s}{dt} = - \frac{z_0}{(1-k) z_l^2} \]  

consequently
\[
C(T) = c_p - \frac{z_0}{(1-k)z_L} \frac{L}{a_L} \quad (33)
\]

or introducing in a place of concentration the dependencies (31) we obtain
\[
C(T) = c_p - \frac{L(T_0 - T_p)}{(1-k)(T - T_p)} \quad (34)
\]

In the case of Scheil model one has
\[
f_L = \left( \frac{T_0 - T_p}{T - T_p} \right)^{1/k} \quad (35)
\]

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

One can see that for \(T = T_0\) the liquid state fraction \(f_L = 1\), while when the solidification process goes to the end \(f_L\) in 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: \(c_S = 2.96 \text{ MJ/m}^3 \text{ K}\), \(c_L = 3.07\), \(\lambda_S = 250\) W/mK, \(\lambda_L = 104\), \(L = 990.6 \text{ MJ/m}^3\), \(k = 0.25\), \(T_p = 660^\circ \text{C}\).

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.

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