

SUBSTITUTE THERMAL CAPACITY OF BINARY ALLOYS. REVIEW OF HYPOTHESES

Jarosław Siedlecki, Wioletta Tuzikiewicz

*Institute of Mathematics, Czestochowa University of Technology, Poland
jaroslaw.siedlecki@im.pcz.pl, wioletta.tuzikiewicz@im.pcz.pl*

Abstract. In the paper the problems connected with the mathematical modeling of alloys solidification (macro scale) are presented. The similar lecture was delivered by the authors during the IV Conference on Mathematical Modelling in Physics and Technique, Kleszczów, 28-30 June 2012. In particular the one domain method (fixed domain approach) in which the parameter called 'a substitute thermal capacity' appears will be discussed. The one domain method bases on the Fourier equation describing the thermal processes in the whole conventionally homogeneous casting domain. The substitute thermal capacity (STC) can be defined in the different ways. The first group of definitions results from the differentiation of the function determining the local volumetric solid state fraction in the neighborhood of the point considered, while the second one is based on the direct assumption of the STC form, at the same time this function should fulfill the condition resulting from the change of alloy physical enthalpy during the phase change. The details of these approaches will be presented in the Sections 2 and 3.

Introduction

Let us 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, x denotes the spatial coordinates, t is a time. One can see, that only heat conduction in a casting volume is considered. The energy equation can constitute a base both in a case of macro-scale modeling and a micro/macro one [1-4]. The differences appear at the stage of derivative $\partial f_s / \partial t$ definition.

The typical mathematical model of casting solidification also contains the energy equation for the mould sub-domain, this meaning

$$c_m(T) \frac{\partial T_m(x, t)}{\partial t} = \nabla [\lambda_m(T) \nabla T_m(x, t)] \quad (2)$$

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

On the external surface of mould the 3rd type of boundary condition is, as a rule, accepted

$$-\lambda_m \frac{\partial T_m(x,t)}{\partial n} = \alpha [T_m(x,t) - T_a] \quad (3)$$

where 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

$$-\lambda \frac{\partial T(x,t)}{\partial n} = \frac{T(x,t) - T_m(x,t)}{R(x,t)} = -\lambda_m \frac{\partial T_m(x,t)}{\partial n} \quad (4)$$

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 is of the form

$$\begin{cases} -\lambda \frac{\partial T(x,t)}{\partial n} = -\lambda_m \frac{\partial T_m(x,t)}{\partial n} \\ T(x,t) = T_m(x,t) \end{cases} \quad (5)$$

The initial temperature distribution for $t = 0$

$$t = 0: T(x,0) = T_0(x), \quad T_m(x,0) = T_{m0}(x) \quad (6)$$

is also known.

1. STC as a result of function f_S knowledge

We denote the temperatures corresponding to the beginning and the end of the solidification process as T_L and T_S . The domain bounded by the values T_L , T_S is called a mushy zone. The first group of STC definitions is based on the assumption that the temperature-dependent function f_S in the interval $[T_S, T_L]$ is known, and then

$$\frac{\partial f_S(x,t)}{\partial t} = \frac{df_S}{dT} \frac{\partial T(x,t)}{\partial t} \quad (7)$$

Introducing the formula (7) to the equation (1) one obtains

$$C(T) \frac{\partial T(x,t)}{\partial t} = \nabla [\lambda(T) \nabla T(x,t)] \quad (8)$$

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

Let us introduce the following definition of STC

$$C'(T) = \begin{cases} c_L & T > T_L \\ c_p - L \frac{df_s}{dT} & T_S \leq T \leq T_L \\ c_S & T < T_S \end{cases} \quad (9)$$

where c_L , c_p , c_S are the volumetric specific heats of molten metal, the mushy zone and solid state sub-domains. In this way one can use the equation (8) as the model of thermal processes proceeding in the whole, conventionally homogeneous, casting domain. The function f_s should fulfill the 'natural' conditions this means $f_s(T_L) = 0$ and $f_s(T_S) = 1$.

The formulated above conditions assures the function of the type

$$f_s(T) = \left(\frac{T_L - T}{T_L - T_S} \right)^n \quad (10)$$

and then

$$\frac{df_s(T)}{dT} = -\frac{n}{T_L - T_S} \left(\frac{T_L - T}{T_L - T_S} \right)^{n-1} \quad (11)$$

Finally

$$C'(T) = c_p - \frac{L}{T_L - T_S} n \left(\frac{T_L - T}{T_L - T_S} \right)^{n-1} \quad (12)$$

or denoting $L/(T_L - T_S) = c_{sp}$ (a spectral latent heat) one has

$$C(T) = c_p + c_{sp} n \left(\frac{T_L - T}{T_L - T_S} \right)^{n-1} \quad (13)$$

It is easy to check that

$$\int_{T_S}^{T_L} \left[c_p + c_{sp} n \left(\frac{T_L - T}{T_L - T_S} \right)^{n-1} \right] dT = c_p (T_L - T_S) + L \quad (14)$$

In particular for $n = 1$ one has

$$C(T) = c_p + \frac{L}{T_L - T_S} = c_p + c_{sp}, \quad T \in [T_S, T_L] \quad (15)$$

One can see that the linear course of f_s leads to the constant value of a thermal capacity of a mushy zone sub-domain. Assuming additionally the constant values of c_s and c_l , one obtains the staircase function as an approximation of $C(T)$.

In Figure 1 the course of STC resulting from (15) is marked [5].

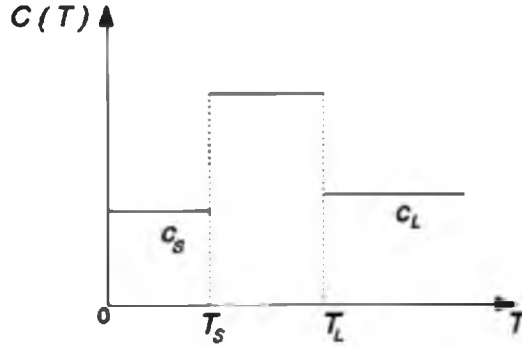


Fig. 1. The course of STC (equation (15))

The substitute thermal capacity shown in Figure 1 is discontinuous. This fact may be disadvantageous from the numerical view-point and the smoothing procedures corresponding to the STC courses shown in Figure 2 can be applied.

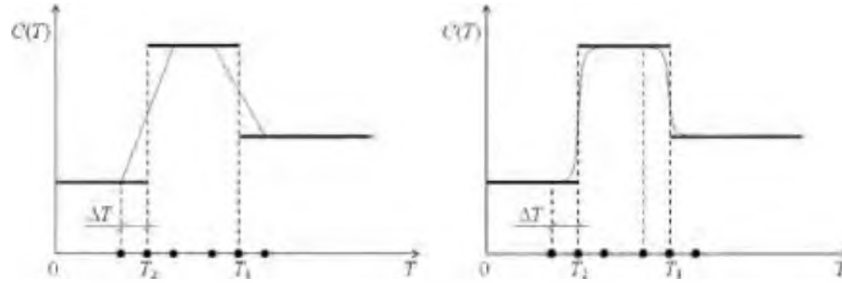


Fig. 2. Smoothing of STC

In paper [6] the definitions of STC resulting from the simple macrosegregation models are presented. In particular, for two successive time levels t and $t+\Delta t$ we have the following form of volume balance

$$V_s(t) z_s(t) + V_L(t) z_L(t) = V_s(t + \Delta t) z_s(t + \Delta t) + V_L(t + \Delta t) z_L(t + \Delta t) \quad (16)$$

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 3 [6]. The values of V_s, V_L and z_s, z_L for time $t + \Delta t$ we can find using the Taylor series

$$V_s(t + \Delta t) = V_s(t) + \frac{dV_s}{dt} \Delta t \quad (17)$$

etc.

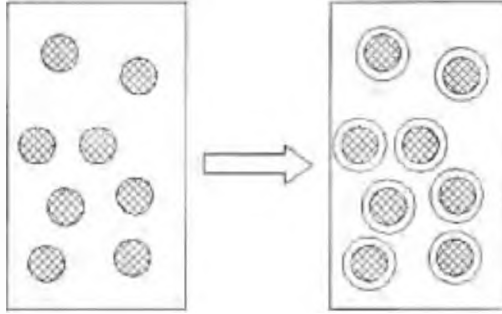


Fig. 3. The change of global $V_s(t)$

Now, the balance (16) takes a form

$$V_s \frac{dz_s}{dt} + \frac{dV_s}{dt} z_s + V_L \frac{dz_L}{dt} + \frac{dV_L}{dt} z_L = 0 \quad (18)$$

or

$$f_s \frac{dz_s}{dt} + \frac{df_s}{dt} z_s + f_L \frac{dz_L}{dt} + \frac{df_L}{dt} z_L = 0 \quad (19)$$

Introducing the partition coefficient $k = z_s/z_L$ and the dependence $f_s = 1 - f_L$ one has

$$\frac{df_L}{dz_L} + \frac{f_L}{z_L} = -\frac{k}{1-k} \cdot \frac{1}{z_L} \quad (20)$$

The equation (20) should be solved using the condition $z = z_0 : f_L = 1$. The solution of equation (20) is of the form

$$f_L = \frac{z_0 - kz_L}{(1-k)z_L} \quad (21)$$

This result corresponds to the well known lever arm model. If the straight lines determining the dependencies $T_s(z_s)$ and $T_L(z_L)$ are of the form

$$\begin{aligned} T_L &= T_p + a_L z_L \\ T_s &= T_p + a_s z_s \end{aligned} \quad (22)$$

(T_p is a solidification point of pure metal) then

Because

$$\frac{df_L}{dT} = \frac{df_L}{dz_L} \frac{dz_L}{dT} = -\frac{z_0}{(1-k)z_L^2} \cdot \frac{1}{a_L} \quad (23)$$

therefore

$$C(T) = c_p + \frac{L(T_0 - T_p)}{(1-k)(T - T_p)^2} \quad (24)$$

We can also assume that the derivative $dz_S/dt = 0$ and then (after the simple mathematical manipulations) one obtains the other form of equation (19)

$$\frac{df_S}{dt} z_S + f_L \frac{dz_L}{dt} - \frac{df_L}{dt} z_L = 0 \quad (25)$$

or

$$\frac{df_L}{f_L} = -\frac{dz_L}{(1-k)z_L} \quad (26)$$

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

$$f_L = \left(\frac{z_0}{z_L} \right)^{1-k} \quad (27)$$

The last equation corresponds to the Scheil model. In which case

$$C(T) = c_p + \frac{L}{(1-k)(T_p - T_0)} \left(\frac{T_p - T_0}{T_p - T} \right)^{\frac{2-k}{1-k}} \quad (28)$$

2. STC - direct approach

The 'start point' of the considerations presented below is the formula

$$\int_{T_S}^{T_L} C(T) dT = c_p(T_L - T_S) + L \quad (29)$$

resulting from the change of physical enthalpy from T_S to T_L .

So, in the paper [7] and lecture [8] the concept of 'broken line' STC approximation has been presented - Figure 4.

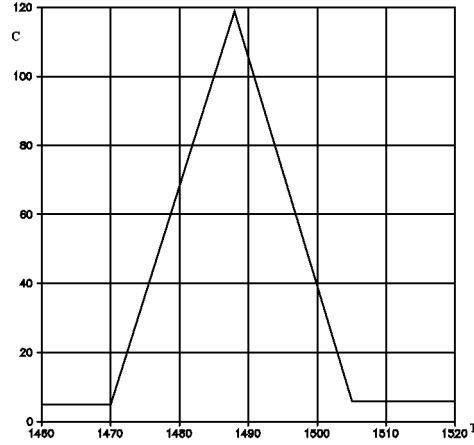


Fig. 4. Course of STC

If T_M denotes a certain value of temperature from the interval $[T_N, T_L]$ then for interval $[T_N, T_M]$

$$C(T) = c_N + \frac{c_{\max} - c_N}{T_M - T_N} (T - T_N) \quad (30)$$

while for $[T_M, T_L]$

$$C(T) = c_L + \frac{c_{\max} - c_L}{T_M - T_L} (T - T_L) \quad (31)$$

Condition (29) leads to the following dependence

$$\frac{c_N + c_{\max}}{2} (T_M - T_N) + \frac{c_L + c_{\max}}{2} (T_L - T_M) = L + c_p (T_L - T_N) \quad (32)$$

In the last equations c_{\max} is the maximum value of thermal capacity. After the simple mathematical manipulations one obtains

$$c_{\max} = \frac{2L + c_L (T_M - T_N) + c_N (T_L - T_M)}{T_L - T_N} \quad (33)$$

The methods of sensitivity analysis show that the choice of T_M is not essential and the Authors of the paper [7] propose to assume the arithmetic mean of interval $[T_N, T_L]$.

Now, the other approximation of STS will be presented (e.g. [3]). For the interval between the border temperatures the parameter discussed is assumed in the form

$$C(T) = c_S + (c_{\max} - c_S) \frac{T - T_S}{T_L - T_S} \quad (34)$$

where c_S is the volumetric specific heat of solid. The value of c_{\max} is show in Figure 5.

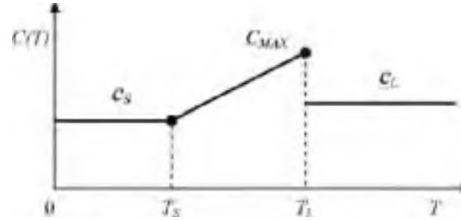


Fig. 5. Linear function $C(T)$

Using the condition (29) one has

$$\int_{T_S}^{T_L} \left[c_S + (c_{\max} - c_S) \frac{T - T_S}{T_L - T_S} \right] dT = c_P (T_L - T_S) + L \quad (35)$$

and the parameter c_{\max} can be found using the equation

$$\frac{1}{2} (T_L - T_S) (c_{\max} + c_S) = c_P (T_L - T_S) + L \quad (36)$$

The very attractive proposition is presented, among others, in the paper [9]. The course of STC is approximated by the polynomial of 4th degree. The coefficients of this function are assumed in such a way that to obtain the continuous and differentiable function, at the same time the condition (29) is also fulfilled.

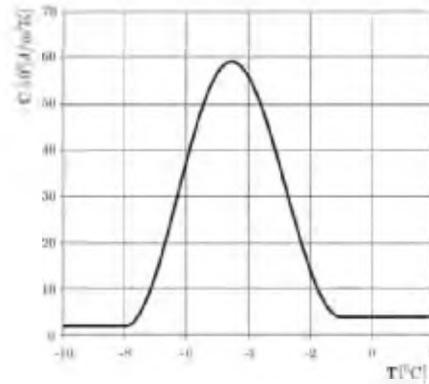


Fig. 6. The course of STC (biological tissue)

In Figure 6 the course of STC for biological tissue is shown. This parameter is used in a case of numerical modeling of the cryosurgery treatments.

Conclusions

The different versions of substitute thermal capacity definitions presented in this paper can be used at the stage of alloys solidification modelling. The formulas correspond to the cases of typical binary alloys and for instance, are not suitable for modelling of cast iron solidification (because of more complex course of the process). The testing computations show that the results of computations using the different hypotheses concerning the STC are similar ones. According to the authors the best hypotheses (from the physical point of view) result from the assumption of coupled thermal and macrosegregation phenomena.

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