Evaluation of interphase boundaries dynamics at the contact of melt with solid material

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Abstract. The results of mathematical modeling of the thermal processes that occur on contact of the melt with a layer of polymer material located on the surface of the hollow microspheres are presented. Dependencies that allow estimating the melting time of the given layer and other parameters of interest in the production of articles from syntactic materials were obtained.

1. Introduction
A set of hollow microspheres with the layer of the solid polymeric material on their surface is considered. It is assumed that the thickness of this layer is the same, the microspheres are tightly packed, at the initial time the temperature of the coated microspheres material is equal to $\Theta_0$. For some time $\tau_n$, the space between the spheres is filled with the melt of the same material as the coating material. The dynamics of the spheres heating and the movement of the interphase boundary starting with the time $\tau_n$ is estimated, provided that the time $\tau_n$ is small, at filling the voids the spheres’ temperature remains equal to $\Theta_0$, the average temperature of the melt is $\Theta_1$. A periodicity cell including a coated microsphere and a melt layer also having a spherical shape with an effective radius $R_e$ is sorted out. Figure 1 shows the corresponding calculation scheme. Here 1, 2, 3, 4 – the gas cavity, the microsphere shell, the polymer coating layer, the conditional layer of polymer melt; $R_0$, $R_1$, $R_c$ – the gas cavity radius, the outer radius of the microsphere shell, the coating surface radius.

2. Body text
In the case of axial symmetry of thermal fields in the absence of internal sources – heat sinks, gas flow in the cavity, melt flow the non-stationary heat transfer in the elements of the considered system is described by the equations:

$$\frac{\partial \Theta}{\partial \tau} = a_i \left( \frac{\partial^2 \Theta}{\partial R^2} + \frac{2}{R} \frac{\partial \Theta}{\partial R} \right),$$

where $\Theta_i$ – the temperature of the substance in the $i$-th area ($i = 1, 2, 3, 4$), $a_i = \lambda_i / (\rho_i \cdot c_i)$ – temperature diffusivity coefficient of the material of the corresponding medium; $\rho_i$, $\lambda_i$, $c_i$ – density, thermal conductivity coefficient, specific heat, $\tau$ – time.
At time $\tau = \tau_n$ the temperatures of the gas, the microsphere shell, and the coating

$$\Theta_i(R, \tau_n) = \Theta_j(R, \tau_n) = \Theta_0,$$  

(2)

the melt layer temperature

$$\Theta_f(R, \tau_n) = \Theta_f.$$  

(3)

The boundary conditions have the form:

$$R = 0: \frac{\partial \Theta_i}{\partial R} = 0 \quad \text{(symmetry condition);}$$  

(4)

$$R = R_0: \Theta_i = \Theta_2, \quad \lambda_1 \frac{\partial \Theta_i}{\partial R} = \lambda_2 \frac{\partial \Theta_2}{\partial R} \quad \text{(ideal thermal contact);}$$  

(5)

$$R = R_1: \Theta_2 = \Theta_3, \quad \lambda_2 \frac{\partial \Theta_2}{\partial R} = \lambda_3 \frac{\partial \Theta_3}{\partial R}.$$  

(6)

Taking into account the fact that the coating and melt materials are the same (at a certain temperature $\rho_3 = \rho_4, \lambda_3 = \lambda_4, c_3 = c_4$) layers 3 and 4 will be considered as one layer with its thermophysical properties characterized by the parameters $\rho, \lambda$ and $c$. Inside this layer, an interphase surface located between the solid material and its melt is marked out. The motion equation of this surface is written as:

$$R_s = R_s(\tau), \quad R_s(\tau_n) = R_{\lambda};$$

with $R = R_s, \Theta = \Theta_s,$

$$\left(\lambda \frac{\partial \Theta}{\partial R}\right)_{R_s=0} = \left(\lambda \frac{\partial \Theta}{\partial R}\right)_{R_s=0} + \rho L v.$$  

(7)

Here $\Theta_s$ – phase transition temperature, $L$ – latent heat of melting, $v = \frac{dR_v}{d\tau}$ – motion speed of the melt front (crystallization).

At the fictitious boundary $R = R_{\lambda},$ we assume:

$$\frac{\partial \Theta}{\partial R} = 0,$$  

(8)

which means that there is no heat exchange with the medium surrounding the selected periodicity cell.

Formulated in this way the thermo-conjugate problem (1) – (8) can be solved numerically. However, for engineering practice the analytical dependencies are useful. In order to obtain them, we simplify this task for this purpose along the radius-vector $R$ we distinguish a prism including the shell
material of the microsphere, solid and molten polymer. In this case, the calculation scheme takes the form shown in figure 2.

\[ \frac{\partial \Theta}{\partial \tau} = a_t \frac{\partial^2 \Theta}{\partial x^2} \]  

(9)

in the polymeric material \((x_t \leq x \leq x_e)\)

\[ \frac{\partial \Theta}{\partial \tau} = a_o \frac{\partial^2 \Theta}{\partial x^2} \]  

(10)

Here, \( \Theta_s = \Theta_s(x, \tau) \), \( \Theta = \Theta(x, \tau) \) – the temperature in the shell, polymeric material \( a_s = \lambda_s / (\rho_s c_s) \) \((\rho_s \equiv \rho_2, \lambda_s \equiv \lambda_2, c_s \equiv c_2)\), \( a_o = \lambda / (\rho c) \).

At time \( \tau = 0 \)

\[ \Theta_s(x, 0) = \Theta_o \ (x_0 \leq x \leq x_1), \ \Theta(x, 0) = \Theta_o \ (x_1 < x < 0), \]  

\[ \Theta(x, 0) = \Theta_i \ (0 < x < x_e). \]  

(11)

Considering that the gas in the microsphere cavity conducts heat poorly, there is no convective heat transfer, at the boundary \( x = x_0 \) we write:

\[ \frac{\partial \Theta_s}{\partial x} = 0. \]  

(12)

Provided an ideal contact in the contact plane of the polymeric material and the microsphere shell

\[ x = x_i : \Theta_s = \Theta, \ \lambda_s \frac{\partial \Theta}{\partial x} = \lambda \frac{\partial \Theta}{\partial x}. \]  

(13)

At a movable interphase boundary (phase-transition front) \( x_e = x_e(\tau) \):

\[ \Theta(x_e - 0, \tau) = \Theta(x_e + 0, \tau) = \Theta_s. \]  

\[ \left( \lambda \frac{\partial \Theta}{\partial x} \right)_{x_e-0} = \left( \lambda \frac{\partial \Theta}{\partial x} \right)_{x_e-0} + \rho Lv(\tau). \]  

(14)

Finally, for \( x = x_e \) in accordance with (8) we have

\[ \frac{\partial \Theta}{\partial x} = 0. \]  

(15)

The problem (9) – (15) can be slightly simplified if we take into account the fact that the microsphere shell thickness \( h_s = x_e - x_0 \) is very small its material has a high thermal conductivity. As a result, considering the shell layer as a thermally thin body assuming that its average temperature \( \Theta_s \): \( \Theta_s + \alpha \tau \) where \( \alpha \) is the average heating rate of a given layer at the boundary \( x = x_1 \), instead of (13) we obtain condition
\[ \lambda \frac{\partial \Theta}{\partial x} + \alpha \rho c \gamma h = \beta \gamma. \]  

(16)

If we further assume that the value \( \beta_0 = \beta_0(\tau) \) is small, the microsphere shell from scheme in figure 2 can be eliminated thereby converting the problem (9) – (15) to the problem of integrating the heat transfer equation (10) in a polymer material layer under the initial condition

\[ \Theta(x, 0) = \begin{cases} 
\Theta_0(x) & \text{for } x \leq x < 0; \\
\Theta_1(0) & \text{for } 0 < x \leq x_c.
\end{cases} \]  

(17)

and boundary conditions (16), (14) and (15).

The problem represented by the relations (10), (16), (17), (14) and (15), many similarities with the problems considered in [1, 2]. From the results of their numerical solution under the condition of thermal insulation at the ends of the computational domain it follows that the function \( \gamma \approx \gamma(\tau) \) can approximately be written in the form:

\[ \gamma = \alpha \gamma_0(\tau - \tau_m)^2, \]  

(18)

where \( \alpha_m \) – the maximum displacement of the interphase boundary towards the melt due to its cooling on contact with solid material, \( \tau_m \) – the time point when the boundary motion reverses it begins to move in the direction opposite to the \( 0x \) axis direction. Since at time \( \tau = 0 \), \( x = 0 \), the coefficient

\[ \alpha_m = \frac{x_m}{\tau_m}. \]  

(19)

Note that the value of \( x_m \) can be estimated by referring to the heat conservation equation of the layer under consideration during the time \( \tau_m \). In this case, it is necessary to take into account that heat losses through the surfaces \( x = x_1 \) and \( x = x_e \) are absent. Approximately

\[ x_m = 0.5c(h_c(\Theta_c - \Theta_1) + 0.5c(\Theta_1 - \Theta_c))/L - 0.5c(\Theta_1 - \Theta_0)) \]  

(20)

\( h_c \) – the thickness of the polymer coating layer).

Further, we require that

\[ x_m : 0.5\delta_m \sqrt{\tau_m}, \]  

(21)

where \( \delta_m \) – an additional parameter characterizing the velocity \( v_0 \) of the interphase boundary at the initial time,

\[ \delta_m = \sqrt{\tau_m}. \]  

(22)

It is easy to make sure [3, 4] that in the region occupied by the melt \( x > x_m \),

\[ \Theta = \Theta(x, \tau) = \Theta_0 + C_1 \left(1 + \Phi \left(\frac{x}{2\sqrt{\pi}a\tau}\right)\right); \]  

(23)

in the solid phase \( x < x_m \)

\[ \Theta = \Theta(x, \tau) = \Theta_0 + C_0 \left(1 - \Phi \left(\frac{x}{2\sqrt{\pi}a\tau}\right)\right). \]  

(24)

Here \( C_0, C_1 \) are the integration constants found from the condition that the ambient temperature at the front of the phase transition of the layers to the left and right of it is equal to \( \Theta_c \);

\[ \Phi(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-u^2) \, du \]  

– the probability integral.

Hence, if \( x_m = 2\sqrt{\pi}a\tau \), then

\[ C_0 = \left((\Theta_c - \Theta_0)/(1 - \Phi(\gamma))\right), \quad C_1 = \left((\Theta_1 - \Theta_c)/(1 + \Phi(\gamma))\right). \]  

It should be noted that the solutions (23) and (24) are valid for infinitely extended regions occupied by the melt and solid material. At the same time, they approximate the temperature field in the vicinity of the interphase boundary quite well. The parameter \( \gamma \) is determined from the heat balance equation on it:
\[ \lambda C_i(\gamma) \exp(-\gamma^2) = \lambda C_i(\gamma) \exp(-\gamma^2) - \sqrt{\pi} \rho a L \gamma. \]  
\tag{23}

For small \( \gamma \) approximately \( \Phi(\gamma) \approx \frac{2}{\sqrt{\pi}} \left( \gamma - \frac{\gamma^3}{3} \right) \), consequently the coefficients

\[ C_0 \approx (\Theta_s - \Theta_t) (1 + \frac{2}{\sqrt{\pi}} (\gamma - \frac{\gamma^3}{3})), \quad C_1 \approx (\Theta_t - \Theta_i) (1 - \frac{2}{\sqrt{\pi}} (\gamma - \frac{\gamma^3}{3})). \]  
\tag{24}

After substituting these values of \( C_0, C_1 \) into equation (23) as a result of a number of transformations to estimate the parameter \( \gamma \), we obtain the formula:

\[ \gamma = \sqrt{\pi c} (2 \Theta_s - \Theta_t - \Theta_t) / (\pi L + 2c(\Theta_t - \Theta_i)). \]  
\tag{25}

From this formula, it is clear that the moving velocity of the interphase boundary will decrease with a decrease of the specific heat and an increase of the latent heat of the material melting. Indeed, with a decrease of the heat capacity with other indices being constant the thermal diffusivity increases, and the heat dissipates faster. If the latent heat of melting increases, more energy is required to overcome intermolecular bonds.

Using the obtained solutions, we estimate the magnitude of the maximum displacement of the interphase boundary \( x_m \). Since at \( \tau = \tau_m \) the boundary velocity \( v(\tau_m) = 0 \) from (14) after substitution of the functions (21) and (22) into this relation, taking into account the dependence \( \gamma_m = 0.5x_m / \sqrt{a\tau_m} \) we find:

\[ x_m = \sqrt{\pi a \tau_m} (2\Theta_s - \Theta_t - \Theta_t) / (\Theta_0 - \Theta_t). \]  
\tag{26}

Comparing formulas (20) and (26) we define the parameter \( \delta_m \):

\[ \delta_m = 2\sqrt{\pi a} (2\Theta_s - \Theta_t - \Theta_t) / (\Theta_0 - \Theta_t). \]  
\tag{27}

Due to the fact that in accordance with the technological requirements the initial movement of the interphase boundary must be reversed in such a way that the polymer coating layer would melt we limit the value of \( x_m \) setting \( x_m = 0.5x_e \).

Hence we obtain the estimate of the time \( \tau_m \):

\[ \tau_m = (x_e / \delta_m)^2. \]

At the time \( \tau = 2\tau_m \) the interphase boundary will return to its original position \( (x_e = 0)\), and the coating material will begin to melt. According to formula (18) the interphase boundary will overcome the distance \( h_s \) in time \( \tau_c = \tau_m \left( \sqrt{1 + \frac{h_s}{x_m}} - 1 \right) \). Therefore, the total execution time of the operation \( \tau_0 = 2\tau_m + \tau_c \).

3. Conclusions

Thus, having the thermophysical parameters of the contacting media, given the geometric dimensions, using the obtained dependencies it is possible to estimate the dynamics of the interphase boundary motion, determine the run-time of the technological operation, thereby minimizing the risks of the appearance of defects [5, 6].

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