Mathematical model of the component mixture distribution in the molten cast iron during centrifugation (sedimentation)

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Mathematical model of the component mixture distribution in the molten cast iron during centrifugation (sedimentation)

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Abstract. For the development and management of the manufacturing processes of axisymmetric articles with compositional structure by centrifugal casting method [1,2,3,4] is necessary to create a generalized mathematical model of the dynamics of component mixture in the molten cast iron during centrifugation. In article, based on the analysis of the dynamics of two-component mixture at sedimentation, a method of successive approximations to determine the distribution of a multicomponent mixture by centrifugation in a parabolic crucible is developed.

1. Introduction

Establishing regularities of structure formation in cast iron in conditions of forced heat and mass transfer by varying the temperature and time parameters of the melting and crystallization is not only the subject of theoretical interest, but also the basis for the development of new manufacturing processes of axisymmetric products with compositional structure by the method of centrifugal casting by centrifugation of the melt. One of the stages of research includes the development of a mathematical model of the transfer and distribution of mixture components in the iron cast melt during centrifugation.

Lamm equation [6], which describes the process of diffusion and sedimentation of substances have been widely used for the study of macromolecules with the aid of analytical ultracentrifugation [6, 7, 8, 9, 10].

To develop mathematical model for assessing the distribution of components in the molten cast iron during centrifugation process, we should consider the known equations describing the process of transfer of matter in the centrifuge cell with diffusion and sedimentation for 2-component mixture [5].

2. The basic part

We shall assume that at the initial time $\tau_0$ all the mixture components are distributed evenly throughout the volume of the filled crucible $V_0$, have the same temperature $T_0$ and the weight of all components is $M_0$. Let the in the initial time $\tau_0$ mass concentration of the components of mixture are given $C_k^0 (\kappa = \bar{1}, \bar{n})$, density of all components $\rho_k^0 (\kappa = \bar{1}, \bar{n})$. In general, $\rho_k$ are functions of temperature $T$ in $\rho_k^0 = \rho_k^0 (T_0)$, where $T_0$ – the temperature of the mixture at $\tau=\tau_0$.

Then, the average density of the mixture $\rho_0$ can be determined by the formula...
\[ \rho_k^0 = \frac{M_0}{V_0}. \quad (1) \]

When centrifuging molecules or particles move under the influence of artificial inertial force directed perpendicularly to the axis of rotation.

We assume, following [5] that the mixture consists of two components. As a standard velocity of the interface \( U \), we accept the change of the radial coordinate \( \frac{dr_{cp}}{d\tau} \) at the midpoint.

Speed value \( U \) can be represented as:

\[ U = \frac{dr_{cp}}{d\tau} = \omega^2 r_s. \quad (2) \]

Where \( \omega \) - the angular velocity of rotation, rev / minute; \( r \) - distance to the axis of rotation, m; \( s \) – sedimentation constant characterizing, as it follows from the equation itself, the rate of deposition of particles per unit of centrifugal acceleration \( \omega^2 r \). The solution of this equation is easy, if you know the sedimentation constant \( s \).

Unfortunately, this constant must be determined by getting the experimental dependence \( \ln \left( \frac{r_{cp}(\tau)}{r_{cp}(\tau_0)} \right) \) of the equation. In the case of multicomponent mixtures more subtle experimental methods are required.

Process of material transportation in the centrifuge is described by Lamm equation [2] which for a radial sector of the cell can be written as:

\[ \left( \frac{dC}{d\tau} \right)_r = -\frac{1}{r} \left[ \frac{d}{dr} \left( \omega^2 r_s C - Dr \left( \frac{dC}{dr} \right)_\tau \right) \right], \quad (3) \]

wherein \( \left( \frac{dC}{d\tau} \right)_r, \left( \frac{dC}{dr} \right)_\tau \), - the concentration function derived (kg / l) at constant values \( r \) and \( \tau \) correspondingly, \( D \) - the diffusion coefficient [m^2/c], \( s \) - sedimentation constant characterizing the particle sedimentation rate per unit centrifugal acceleration \( \omega^2 r \). This equation, as shown in [6,7] has not, in general, the exact analytical solution. Nevertheless, for two extreme cases there are the exact solutions: when \( D = 0 \) the (lack of diffusion) and \( s = 0 \) (no sedimentation). Since we are interested in the case when the effect of diffusion comparing to inertial forces is small, we consider the solution of equation (3) with \( D = 0 \).

Taking into account Fick equation, which describes the process of diffusion and sedimentation of interface in an infinite stream in the direction which is perpendicular to the rotation axis OX [6].

When \( D = 0 \), we obtain \( x = x_0 \exp(s\omega^2\tau) \),

\( x_0 \) - where - the interface (meniscus), and taking into account (1), we find

\[ \begin{cases} 
C(x, \tau) = 0; & \text{при } x \in (x_0, x_\tau) \\
C(x, \tau) = C_0 \exp(-2s\omega^2\tau); & \text{при } x \in (x_\tau, x_0) 
\end{cases} \quad (4) \]

where \( x_0 \) - the initial coordinate of mixture interface (meniscus), m;
$x_0$ - coordinate of the crucible bottom, m; $C_0$ - initial concentration, kg/l.

Distribution of concentration over time in this case, has the plateau with a constant concentration. The essential fact in this solution is that over time the particles of the corresponding component concentrate on the side surface of the crucible with a higher density and the lower density components are distributed along the side surface of the preceding components.

Taking into consideration that the limit solution of Lamm equation (4) and the fact that the assigned task of the components distribution in volume where $\tau \to \infty$ does not require knowledge of the prehistory of the process, you can reduce it to a fairly simple algorithm. Suppose that the form of the crucible is defined by the equation:

$$y = \frac{H_* x^2}{R_*^2},$$

(5)

where $R_*, H_*$ - constants that are the coordinates of an arbitrary point on the boundary section.

We order the components of the mixture in ascending given when $\tau_0$ densities $\rho_1 < \rho_2, <... < \rho_n$ and define the corresponding mass concentration $C_k^0 (k = 1,n)$ of components of the mixture at the initial time $\tau_0$.

While centrifugation component molecules move under the influence of artificial gravitational field and after a certain time, according to a particular solution of the equation Lama (3), will be located in layers.

We assume that the rotational speed of the crucible is bounded both above and below so that the contents of the crucible did not form the gaps near the axis and inertial forces exceed gravity.

To determine the limits of mixture components developed a method of successive approximations.

For the particular case of three-component mixture $Fe-C-Si$ at concentrations equal to $C, Fe-92.45\%; C-5.1\%; Si-2.45\%$, total mass $M_0=1002$ and a predetermined shape of the crucible $H_*=12 cm$, $R_*=3.6 cm$ calculations have been made the results of which after three iterations are shown in table 1.

Table 1
Table of calculations results

| Iteration $\tau_0$ | $r_1$ (cm) | $r_2$ (cm) | $r_3$ (cm) | $H_1$ (cm) | $H_2$ (cm) | $H_3$ (cm) |
|-------------------|------------|------------|------------|------------|------------|------------|
| 0                 | 0.692      | 0.8368     | 1.8710     | 2.974      | 2.974      | 3.150      |
| 1                 | 0.685      | 0.8283     | 1.8517     | 2.986      | 2.992      | 3.062      |
| 2                 | 0.690      | 0.8343     | 1.8651     | 2.986      | 2.985      | 3.018      |

Here $r_k, H_k$ coordinates of the upper boundary point of "k"-th mixture ($k = 1,3$).
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