Calculation of the distribution of temperature in the form based on magnesium oxide for the casting of titanium products

N F Kashapov, I G Dautov, L A Tkachenko, S A Fadeev and L R Shaidullin

1 Kazan Federal University, 18 Kremlyovskaya str., Kazan 420008, Russia
2 Kazan National Research Technical University named by A.N.Tupolev, 420111, K.Marx str., 10, Kazan, Russia
3 Institute of Mechanics and Engineering, Subdivision of the Federal State Budgetary Institution of Science «Kazan Scientific Center of the Russian Academy of Sciences», 2/31, Lobachevsky str, 420111, Kazan, Russia

E-mail: sergey_fadeev@kpfu.ru

Abstract. Calculations of the distribution of temperature in the mold based on magnesite oxide, when casting products from titanium alloys, are presented. It is shown that in the mold based on magnesite oxide it cools down exponentially to ambient temperature.

1. Introduction

In the process of interaction of molten titanium with a mold based on magnesite oxide, a large number of chemical reactions occur, both reversible and irreversible. It is necessary to single out those of them, whose products, if they fall on the “mold-casting” boundary, can lead to the formation of TiO$_2$. The amount of oxygen forming the alpha case layer depends on the time of thermal exposure in a certain temperature range. Thus, knowing the coefficients of thermodiffusion of molecules of compounds containing oxygen and participating in chemical reactions in a titanium melt, it is possible to determine the main causes of the formation of an alpha case layer [1-5].

2. Model and discussion

The mold cools down in the oven at an ambient temperature of 600 °C, the initial temperature $T_0$ can be set. Heat removal through the gate system is rather small, since the process of melting and cooling of the casting is carried out in a vacuum. In this case, the integral energy luminosity is proportional to the outer area of the object, it can be assumed that in a sufficient distance from the gating system, the heat is removed from the melt through the mold. Assuming that the mold-casting interface is flat, setting the temperature of the molten titanium $T_1 = 1961$ K, for the case of an unsteady heat flux in a solid without internal sources, we consider the equation of the nonstationary temperature field (the Fourier heat equation)

$$\frac{\partial T}{\partial t} = a\nabla^2 T$$

(1)
At the initial time, the temperature at the "mold-casting" boundary $T_1$. The ambient temperature is $T_0$.

We introduce the dimensionless temperature

$$\theta = \frac{T - T_0}{T_1 - T_0}. \hspace{1cm} (2)$$

As a result of the transformation of equation (1), we obtain

$$\frac{\partial \theta}{\partial t} = a \nabla^2 \theta \quad \text{или} \quad \frac{\partial \theta}{\partial \text{Fo}} = \nabla^2 \theta \hspace{1cm} (3)$$

where $a$ is the thermal diffusivity.

We seek the solution of equation (3) in the form of a product of two functions, one of which is related only to the coordinate, the other only with time

$$\theta = \varphi(\text{Fo})\psi(\xi), \hspace{1cm} (4)$$

where $\text{Fo} = \frac{at}{\delta^2}$ is the function of the Fourier criterion, $\xi = \frac{x}{\delta}$ is the coordinate function, and $\delta$ is the thickness of the plate. Substituting (4) into (3), we obtain

$$\varphi(\text{Fo})\psi(\xi) = \varphi(\text{Fo})\nabla^2 \psi(\xi) \hspace{1cm} (5)$$

In order for expression (4) to satisfy equation (3), it is necessary that the functions $\varphi$ and $\psi$ satisfy the condition:

$$\frac{\varphi(\text{Fo})}{\varphi(\text{Fo})} = \frac{\nabla^2 \psi(\xi)}{\psi(\xi)} = -\beta^2 \hspace{1cm} (6)$$

Also, in order for function (4) to be a solution of equation (1), equality (5) must be satisfied identically, that is, for all values of independent variables $0 < x < \delta$, $t > 0$. Therefore, fixing, for example, some value of $x$ and changing $t$ (or vice versa), we find that the right and left parts of (5) retain a constant value $-\beta^2$ when changing their arguments (the values of such a parameter are called eigenvalues).

We introduce the initial conditions

$$\theta = 1, \text{Fo} = 0. \hspace{1cm} (7)$$

The boundary conditions have the form

$$\left(\frac{d\theta}{d\xi}\right)_{\xi=0} = 0, \quad \xi = 0, \hspace{1cm} (8)$$

$$-\lambda_r \left(\frac{\partial \theta}{\partial x}\right)_{x=\delta} = \alpha(T - T_\infty)_{x=\delta}. \hspace{1cm} (9)$$
A boundary condition of the third kind in the dimensionless form is written as

\[- \left( \frac{d \theta}{d \xi} \right)_{\xi=0} = Bi(\theta)_{\xi=1}, \quad (10)\]

Where \( Bi = \frac{\alpha \delta}{\lambda_\gamma} \) - Bio criterion, \( \alpha \) - heat transfer coefficient, \( \lambda_\gamma \) - thermal conductivity coefficient.

We substitute \( \theta = \psi \varphi \) into the boundary conditions (8) and (10), we obtain

\[ \left( \frac{d \psi}{d \xi} \right)_{\xi=0} = 0, \quad \xi = 0, \quad (11) \]

\[- \left( \frac{d \psi}{d \xi} \right)_{\xi=0} = Bi(\psi)_{\xi=1}, \quad (12) \]

In this case, the function \( \psi \) depends only on one variable \( \xi \), then from equation (6) we obtain

\[ \frac{d^2 \psi}{d \xi^2} + \beta^2 \psi = 0. \quad (13) \]

The solution of equation (13) is

\[ \psi = C_1 \cos \beta \xi + C_2 \sin \beta \xi. \quad (14) \]

The condition (11) is satisfied only by the even function, therefore we set

\[ C_2 = 0. \quad (15) \]

We rewrite (14) in the form

\[ \psi = C_1 \cos \beta \xi, \quad (16) \]

we substitute (16) into (12) and obtain

\[ \beta \sin \beta = Bi \cos \beta. \quad (17) \]

The transcendental equation (17) does not have an analytical solution and is solved by the graphical method [2]. It follows from equation (17) that the boundary conditions determine the values of the constants \( \beta_n \), while the constant \( C_1 \) is found by means of boundary conditions.

The function \( \varphi \) depends only on time, then from equation (6) we obtain

\[ \varphi'(Fo) + \varphi(Fo) \beta^2 = 0. \quad (18) \]

A solution of equation (18) is a temperature versus time
\[ \varphi(Fo) = Ce^{-b^2Fo} . \] (19)

Thus, the general solution of equation (3) has the form of a series

\[ \theta = \sum_{i=1}^{\infty} C_i \cos \beta_i \xi e^{-\beta_i^2Fo} . \] (20)

The coefficients \( \beta_i \) increase rapidly with the number of the term of the series, so the more the criterion \( Fo \), the smaller the value of the highest term of the series in comparison with the previous ones. As a result, after some value of \( Fo \), all the terms of the series become negligibly small in comparison with the first term of the series. The technical process of cooling the casting is up to several hours, so the temperature with a higher degree of accuracy can be expressed by a single-term formula

\[ \theta = C_i \cos \beta_i \xi e^{-\beta_i^2Fo} . \] (21)

The constant \( C_i \) is calculated by substituting (21) into the initial conditions (7), then the dimensionless temperature has the form

\[ \theta = 2 \frac{\sin(\beta_i) \cos(\beta_i \xi)}{\beta_i + \sin(\beta_i) \cos(\beta_i)} e^{-\beta_i^2Fo} . \] (22)

We reduce the expression (22) to the dimensional form

\[ T = 2 \frac{\sin(\beta_i) \cos(\beta_i \xi)}{\beta_i + \sin(\beta_i) \cos(\beta_i)} e^{-\beta_i^2Fo} (T_1 - T_0) + T_0. \] (23)

Expression (23) is a solution of the heat equation (1). In the case of a mold based on magnesite oxide \( Bi \approx 860 \), which corresponds to \( \beta_1 = \pi/2 \) [2]. Fig. 1 shows the calculation of the temperature distribution in mold based on magnesite oxide when casting a titanium product.

![Figure 1](image-url)

**Figure 1.** Calculation of temperature distribution in a mold based on magnesite oxide form when casting a titanium product.
When casting products from titanium, a mold based on magnesite oxide heated up to 1961 K (melting temperature of Ti) and, subsequently, it cools down exponentially to the temperature in the furnace. Knowing the temperature distribution in the mold, at each instant of time, and having the thermal diffusion coefficients of the molecules of compounds containing oxygen, it is possible to determine the amount of oxygen diffusing into the casting and participating in the formation of the alpha case layer. This will allow to develop new methods of casting titanium products in a mold based on magnesite oxide, aimed at preventing the formation of an alpha case layer [9-20]. This will lead to a reduction in the labor intensity and cost of the technological process of casting titanium products.

Acknowledgments
This work was funded by the subsidy allocated to Kazan Federal University for the state assignment in the sphere of scientific activities (11.1300.2017/4.6), Presidential Program for State Support of Young Candidates of Sciences (grant no. MK-539.2017.1), and the research grant of Kazan Federal University.

References
[1] Maulilov L A 1962 Physical chemistry and chemistry of silicon (Moscow, High school) p 65
[2] Tkachenko L A 2017 Heat exchange theory (Kazan, Publishing house of Kazan University) p 151
[3] Kutateladze S S 1979 Fundamentals of heat exchange theory (Moscow, Atomizdat) p 416
[4] Kutateladze S S 1990 Heat Transfer and Hydrodynamic Resistance (in Russian) (Moscow, Energoatomizdat Publishing House) p 366
[5] Schlichting H 1974 Boundary layer theory (in Russian) (Moscow, Science) p 711
[6] Kudinov V A, Kartashov E M and Stefanyuk E V 2015 Technical thermodynamics and heat transfer: a textbook for academic baccalaureate (in Russian) (Moscow, Yurayt Publishing House) p 566
[7] Gavrilova V A, Fazlyyyakhmatov M G and Kashapov N F 2013 J. Phys.: Conf. Ser. 479 012010
[8] Saifutdinov A I, Saifutdinova A A, Kashapov N F and Fadeev S A 2016 J. Phys.: Conf. Ser. 669 012045
[9] Kornienko E E, Lapushkina E I, Kuzmin V I, Vaschenko S P, Gulyaev I P, Kartaev E V, Sergachev D S, Kashapov N, Sharifullin S, Fayrushin I 2014 J. Phys.: Conf. Ser. 567 012010
[10] Saifutdinov A I, Fairusih I I and Kashapov N F 2016 JETP Lett. 104 180–185
[11] Luchkin A G, Kashapov N F and Luchkin G S 2013 J. Phys.: Conf. Ser. 479 012019
[12] Hakki A, Kashapov N and Sadikov K 2017 J. Phys.: Conf. Ser. 927 012022
[13] Fayrushin I I, Dautov I G and Kashapov N F 2017 International Journal of Environmental Science and Technology 14 (12) 2555–2560
[14] Zaripov R G, Tkachenko L A and Shaydullin L R 2014 J. Phys.: Conf. Ser. 567 012042
[15] Shaydullin L R 2016 IOP Conf. Ser.: Mater. Sci. Eng. 134 012022
[16] Gubaidullin D A, Kashapov N F, Zaripov R G, Tkachenko L A and Shaydullin L R 2017 J. Phys.: Conf. Ser. 789 012017
[17] Gubaidullin D A, Zaripov R G, Tkachenko L A and Shaidullin L R 2017 High Temperature 55 (3) 469–471
[18] Zaripov R G, Tkachenko L A, Shaidullin L R 2017 Journal of Engineering Physics and Thermophysics 90 (6) 1463–1468
[19] Fadeev S A and Saifutdinov A I 2017 Plasma Physics Reports 43 (11) 1080–1088
[20] Tkachenko L A and Fadeev S A 2017 Acoustical Physics 63 (1) 7–13