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MATHEMATICAL MODEL OF CHARTS MELT VISCOSITY OF THE CaO - SiO_2 - Al_2O_3 – MgO

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Experimentally using electric vibration viscometer and the method of design of experiments on the simplex studied the melt viscosity of the system CaO - SiO_2 - Al_2O_3 - MgO. Developed its mathematical model and computer program that allows calculation of viscosity in the temperature range 1 573 - 1 823 K. Using the model diagrams are constructed in the form of isothermal sections of the tetrahedron on MgO. It is concluded that the use of the model is more efficient than Chart, so it does not require a complex geometric constructions tetrahedron when the viscosity values, and, moreover, can be used in automatic process control in real time.

Keywords: metallurgy, CaO - SiO_2 - Al_2O_3 - MgO system, viscosity, electric conductivity, axial diagram

INTRODUCTION

In the research and production activities is common for evaluation of the properties of slag and metal from the diagrams. They are visible and give the opportunity to choose among the many specific compositions presented. However, there are difficulties in their use. This inability to image plane multicomponent (more than four) systems, insufficient accuracy of removing the charts data by geometric constructions, the impossibility of their use in automatic process control in real time. It seems appropriate to create a mathematical model diagrams when the above-mentioned difficulty is largely removed. Sharing graphic diagrams and mathematical models should help improve the effectiveness of research in this area. This article presents the results of the work in this direction.

RESEARCH METHODOLOGY

The decision of the goal to create a mathematical model requires the use of a common reference data of high accuracy. Analysis of the available data[1 - 8] showed significant differences in viscosity of the same slag at the same temperature due to methodological errors[9 - 11], therefore, it was decided to independently carry out experimental investigations, taking measures to reduce instrument and computational errors. For the above reason, it was decided to independently perform experimental studies viscosity, taking measures to reduce the instrumental and computational errors. To determine the viscosity was chosen amplitude resonant version of the method vibration viscometry. It has high sensitivity and allows to determine the viscosity of the slag in a wide range of values [12].

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RESULTS OF RESEARCHING

For research in the system CaO - SiO_2 - Al_2O_3 - MgO was selected portion encompassing the most common oxide melts domain, cupola, ferroalloy, ceramic and other industries. It was a tetrahedron whose vertices are located in the following areas: the first - on the side of the binary CaO – Al_2O_3 at crystallization at twelve-calcium seven aluminate ($12CaO{\cdot}7Al_2O_3$) with coordinates 48,48 % CaO and 51,52 % Al_2O_3, the second one on the side of the binary CaO – SiO_2 between rankinite ($3CaO{\cdot}2SiO_2$) and pseudowollastonite ($aCaO{\cdot}SiO_2$) with coordinates / %: 52 CaO and 48 SiO_2, in a third one of the ternary eutectic crystallization point with coordinates / %: 9,8 CaO, 19,8 Al_2O_3 and 70,4 SiO_2, and the fourth was in the volume of the tetrahedron and contained / %:12CaO, 19SiO_2, 9Al_2O_3 и 40MgO.

Used on the simplex method of planning, allowing a mathematical model and build diagrams «structure - property» [13, 14]. In this method, the form approximating polynomial is given in advance, and the degree of the polynomial is determined depending on the expected complexity of the response surface. To study four-component system CaO - SiO_2 - Al_2O_3 - MgO was selected fourth degree polynomial.

The total form of the equation for calculating the viscosity versus composition at a fixed temperature as follows.

$$\lg\eta = \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \beta_4x_4 + \beta_{12}x_1x_2 + \beta_{13}x_1x_3 + \beta_{14}x_1x_4 + \beta_{23}x_2x_3 + \beta_{24}x_2x_4 + \beta_{34}x_3x_4 + \gamma_{12}x_1x_2(x_1 - x_2) + \gamma_{13}x_1x_3(x_1 - x_3) + \gamma_{14}x_1x_4(x_1 - x_4) + \gamma_{23}x_2x_3(x_2 - x_3) + \gamma_{24}x_2x_4(x_2 - x_4) + \gamma_{34}x_3x_4(x_3 - x_4) + \sigma_{12}x_1x_2(x_1 - x_2)^2 + \sigma_{13}x_1x_3(x_1 - x_3)^2 +$$

$\sigma_{14}x_1x_4(x_1 - x_4)^2 + \sigma_{23}x_2x_3(x_2 - x_3)^2 + \sigma_{24}x_2x_4(x_2 - x_4)^2 + \sigma_{34}x_3x_4(x_3 - x_4)^2 + \beta_{1123}x_1^2x_2x_3 + \beta_{1124}x_1^2x_2x_4 + \beta_{1134}x_1^2x_3x_4 + \beta_{2234}x_2^2x_3x_4 + \beta_{1223}x_1x_2^2x_3 + \beta_{1224}x_1x_2^2x_4 + \beta_{1334}x_1x_3^2x_4 + \beta_{2334}x_2x_3^2x_4 + \beta_{1233}x_1x_2x_3^2 + \beta_{1244}x_1x_2x_4^2 + \beta_{1344}x_1x_3x_4^2 + \beta_{2344}x_2x_3x_4^2 + \beta_{1234}x_1x_2x_3x_4$ (Eq 1)

where η – viscosity / Pa·s,

β_1, β_2, β_3 and so on - the coefficients of which are calculated from the experimentally found values of viscosity, and are shown in Table 5.

x_1, x_2, x_3 и x_4 – content, respectively pseudocomponents CaO, SiO_2,

Al_2O_3 and MgO in the vertices of the simplex, of a unit.

In planning matrix Central slag composition of the coordinates of pseudo-weight percentage is produced by the formulas:

$CaO = 4\,8{,}48x_1 + 52x_2 + 9{,}8x_3 + 12x_4$, (Eq 2)

$SiO_2 = 4\,8x_2 + 70{,}4x_3 + 39x_4$ (Eq 3)

$Al_2O_3 = 51{,}52x_1 + 19{,}8x_3 + 9x_4$ (Eq 4)

$MgO = 40x_4$ (Eq 5)

When the machine method for finding the viscosity of the expression (1) the system of equations (2) - (5) are solved in a general way with respect to x_1, x_2, x_3 and x_4:

$x_1 = 4{,}28\cdot10^{-6}\cdot MgO + 1{,}516\cdot10^{-2}\cdot Al_2O_3 -$
$-4{,}892\cdot10^{-3}\cdot SiO_2 + 4{,}516\cdot10^{-3}\cdot CaO$, (Eq 6)

$x_2 = -\,3{,}629\cdot10^{-3}\cdot MgO - 1{,}622\cdot10^{-2}\cdot Al_2O_3 +$
$+\,2{,}162\cdot10^{-3}\cdot SiO_2 + 1{,}723\cdot10^{-2}\cdot CaO$, (Eq 7)

$x_3 = -\,1{,}137\cdot10^{-2}\cdot MgO +{,}106\cdot10^{-2}\cdot Al_2O_3 +$
$+\,1{,}273\cdot10^{-2}\cdot SiO_2 - 1{,}175\cdot10^{-2}\cdot CaO$, (Eq 8)

$x_4 = 2{,}5\cdot10^{-2}\cdot MgO$ (Eq 9)

According to the developed method, a known part of slag CaO, SiO_2, Al_2O_3 and MgO by using Equations (6 - 9) are initially values x_1, x_2, x_3 and x_4 that substituting into equation 1, one can determine the viscosity. The crystallization temperature of slag of the logarithm of viscosity versus inverse absolute temperature and applied the same processing techniques to create a mathematical model.

DISCUSSION RESULTS OF RESEARCHING.

Experimental values of viscosity (η) and the crystallization temperature ($T_{cr.}$) served as a basis for calculating said equation (1) the polynomial coefficients. For example, $\beta_1 = \eta_1$; $\beta_2 = \eta_2$; $\beta_3 = \eta_3$; $\beta_4 = \eta_4$; $\beta_{12} = 9/4(\eta_{112} + \eta_{122} - \eta_1\cdot\eta_2)$ and so on [15]. The thus obtained all 35 coefficients for the polynomial viscosity and crystallization temperature are given in Table 5. In accordance therewith, the equation for calculating the viscosity to temperature, such as 1 773K as follows.

$\lg\eta = -\,0{,}195x_1 - 0{,}407x_2 + 1{,}250x_3 + 3{,}000x_4 + 3{,}203x_1x_2 - 0{,}547x_1x_3 - 3{,}719x_1x_4 + 0{,}473x_2x_3 - 7{,}107x_2x_4 - 8{,}215x_3x_4 - 1{,}415x_1x_2(x_1 - x_2) + 4{,}309x_1x_3(x_1 - x_3) + 3{,}373x_1x_4(x_1 - x_4) - 2{,}31x_2x_3(x_2 - x_3) - 2{,}008x_2x_4(x_2 - x_4) + 10{,}838x_3x_4(x_3 - x_4) - 9{,}548x_1x_2(x_1 - x_2)^2 + 10{,}371x_1x_3(x_1 - x_3)^2 - 10{,}707x_1x_4(x_1 - x_4)^2 + 0{,}312x_2x_3(x_2 - x_3)^2 + 3{,}737x_2x_4(x_2 - x_4)^2 - 6{,}636x_3x_4(x_3 - x_4)^2 + 39{,}515\,x_1^2x_2x_3 - 17{,}588\,x_1^2x_2x_4 - 35{,}808\,x_1^2x_3x_4 + 16{,}794\,x_2^2x_3x_4 - 61{,}898\,x_1x_2^2x_3 - 3{,}263\,x_1x_2^2x_4 - 11{,}692\,x_1x_3^2x_4 - 15{,}164\,x_2x_3^2x_4 - 0{,}740\,x_1x_2x_3^2 - 21{,}492\,x_1x_2x_4^2 + 41{,}875\,x_1x_3x_4^2 + 18{,}261\,x_2x_3x_4^2 + 27{,}45\,x_1x_2x_3x_4$ (Eq 10)

The crystallization temperature can be calculated so.

$T_{cr.} = 1\,593x_1 + 1\,793x_2 + 1\,618x_3 + 1\,867x_4 + 320x_1x_2 + 70x_1x_3 + 8x_1x_4 - 330x_2x_3 - 292x_2x_4 - 62x_3x_4 + 0x_1x_2(x_1 - x_2) + 120x_1x_3(x_1 - x_3) - 805{,}33x_1x_4(x_1 - x_4) + 333{,}33x_2x_3(x_2 - x_3) - 1\,018{,}67x_2x_4(x_2 - x_4) + 114{,}67x_3x_4(x_3 - x_4) - 1\,173{,}33x_1x_2(x_1 - x_2)^2 + 2\,866{,}67x_1x_3(x_1 - x_3)^2 - 714{,}67x_1x_4(x_1 - x_4)^2 + 93{,}33x_2x_3(x_2 - x_3)^2 - 773{,}33x_2x_4(x_2 - x_4)^2 - 989{,}33x_3x_4(x_3 - x_4)^2 + 7\,240\,x_1^2x_2x_3 + 138{,}67\,x_1^2x_2x_4 - 1\,597{,}33\,x_1^2x_3x_4 + 1\,1314{,}7\,x_2^2x_3x_4 - 15\,160\,x_1x_2^2x_3 + 1\,658{,}67\,x_1x_2^2x - 2\,362{,}67\,x_1x_3^2x_4 + 8\,688\,x_2x_3^2x_4 + 6\,906{,}67\,x_1x_2x_3^2 - 7\,098{,}67\,x_1x_2x_4^2 + 1\,586{,}67\,x_1x_3x_4^2 - 14\,344\,x_2x_3x_4^2 - 29\,450{,}7\,x_1x_2x_3x_4$ (Eq 11)

Developed models can be used to evaluate the properties of the melts, the following values contoured oxides concentration wt.%: CaO 9,8 - 52,0; SiO_2 0 - 70,4; Al_2O_3 0 - 51,52 and MgO 0 - 40.

Models can be used to visualize the results of calculations by charting. Figures 1 and 2 show an example. Comparison of these diagrams with the most cited in the literature [5 - 7] shows identity stroke contour and match the numerical values of properties in a number of areas.

Describing the overall structure of these diagrams, it can be noted that they can clearly be seen extreme dependence of these properties on the composition. When raising the state diagram and phase diagram of this system can be established that these specific areas are confined to eutectic crystallization and fields of chemical compounds, which confirms the view of the presence in the liquid such as molecules associations undergoing structural transformations during cooling [16,17].

In a number of productions being continuous or periodic monitoring of the chemical composition of the melt. In this case, the model can be used to evaluate their properties in automatic process control.

CONCLUSION

Mathematical models diagrams and charts viscosity melt crystallization temperature of the CaO - SiO_2 - Al_2O_3 - MgO. They allow you to conduct numerical calculations of the unknown quantities by the chemical composition of the melt. Using the model are graphs of viscosity and crystallization temperature. Sharing models and diagrams easier to find the desired compositions for the process. It is possible to use models in automatic process control in real time.

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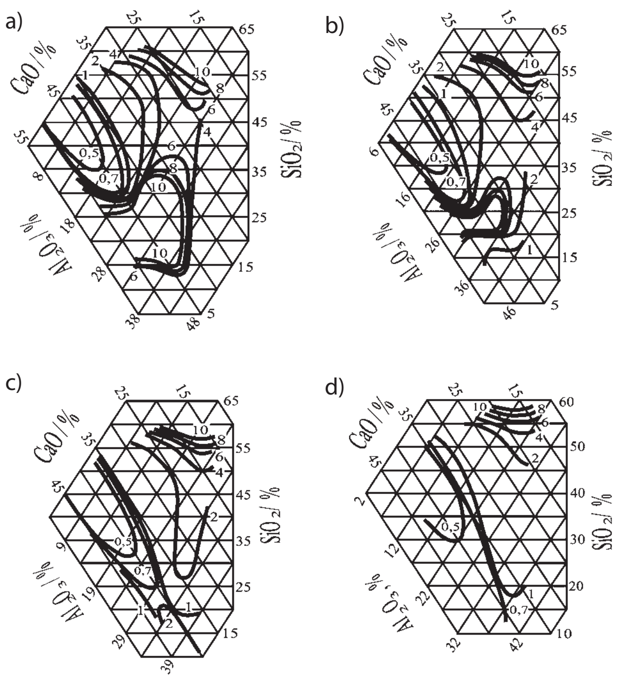

Figure 1 Diagrams the melt viscosity of the system CaO - SiO_2 - Al_2O_3 - MgO with 2 (a), 4 (b), 6 (c) and 8 % MgO (d) at 1 723K.

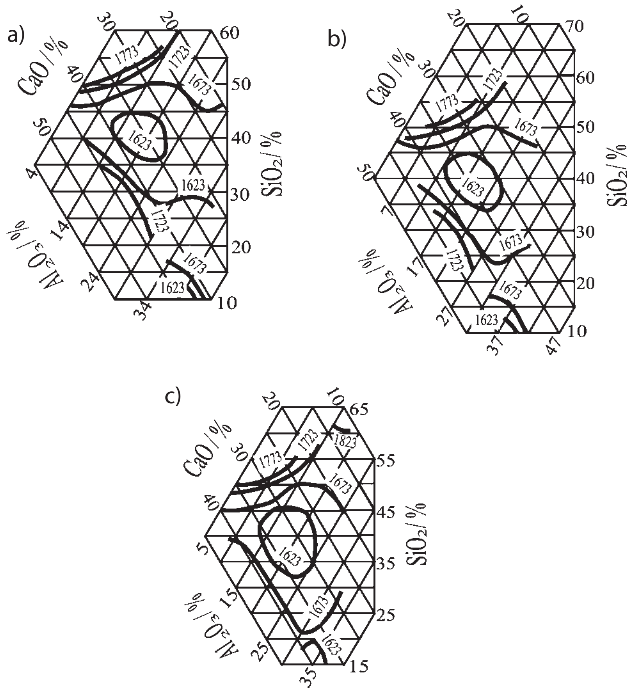

Figure 2 Diagrams the melt crystallization temperature systems CaO - SiO_2 - Al_2O_3 - MgO with 6 % (a), 8 % (b) and 10 % MgO (c).

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Note: The responsible for English language is lector from University.