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MODELING PHYSICOCHEMICAL PROPERTIES OF MOLD SLAG

MODELOWANIE WŁAŚCIWOŚCI FIZYKOCHemiczNYCH ŻUŻLI KRYSTALIZATOROWYCH

This paper deals with the mathematical modeling of physicochemical properties of mold slag such as: viscosity, surface tension, temperature liquidus, basicity. Computer simulation of slag viscosity was made by the Nakamoto structural model. The effect of addition CaF_2 to the mold slag was estimated by using of Urbain model. The results were compared with the results of the experiment. Surface tension for the basic slag composition: $\text{CaO} - \text{SiO}_2 - \text{Al}_2\text{O}_3$ was calculated with using Nakamoto model. The results of calculations indicate that the content of the SiO_2 lowers the surface tension, but increase the content of CaO and Al_2O_3 in the slag increases its value. Calcium fluoride (CaF_2) reduces the viscosity of the slag. The increase in temperature reduces the viscosity of the slag, simultaneously increasing the surface tension.

Keywords: mold slag, viscosity model, surface tension model, range of liquid phase, basicity, computer simulation

Praca zajmuje się modelowaniem właściwości fizykochemicznych żużli krystalizatorowych, takich jak: lepkość, napięcie powierzchniowe, temperatura liquidus, zasadowość. Korzystając z modelu strukturalnego Nakamoto obliczono lepkość żużla. Wpływ dodatku CaF_2 na lepkość określono wykorzystując klasyczny model Urbain'a. Uzyskane z obliczeń wyniki porównano z wynikiem eksperymentu. Korzystając z modelu Nakamoto obliczono napięcie powierzchniowe żużla dla podstawowego układu tlenkowego: $\text{CaO} - \text{SiO}_2 - \text{Al}_2\text{O}_3$. Wyniki symulacji komputerowych wskazują, że zawartość SiO_2 obniża napięcie powierzchniowe żużli, z kolei równoczesne zwiększenie zawartości CaO i Al_2O_3 powoduje wzrost tej wielkości. Wyniki modelowania wskazują, że dodatek CaF_2 oraz wzrost temperatury obniżają lepkość, z kolei podwyższenie temperatury powoduje wzrost napięcia powierzchniowego.

1. Introduction

Mold powders which after melting constitute the mold slags, are composed of oxides with addition of fluorides and granulated carbon. Carbon included in mold slag reacts with oxides of iron present in slag, and, to some extent, poured into the mold with steel. As a result of reaction between carbon and iron oxides the carbon oxide CO is formed, which provides a reducing atmosphere in the crystallizer. Carbon exists in mold slag in the form of fine particles, originating from component – bearing type of graphite, black carbon, coke breeze. The quantity of carbon particles and the contents of structure modifiers: CaF_2 , Na_2O , K_2O , KF , NaF determines the liquidus temperature of mold slag. Studies of the impact of CaF_2 component in mold slag confirm that the introduction of calcium fluoride decreases slag viscosity. The slag viscosity is directly related to chemical composition, and, consequently, the structure of liquid melts. Slag viscosity influences also high temperature reactions in inter-phase region between molten slag and liquid steel [1]. Studies of molten slag structure [2] show that the oxide systems are made of chains and rings of silicate type: $[\text{Si}_3\text{O}_9]^{6-}$ (ring), $[\text{Si}_3\text{O}_{10}]^{8-}$ (chain), $[\text{Si}_3\text{O}_9\text{F}]^{7-}$ (chain). They also contain smaller and simpler silicate constructions,

such as: $[\text{Si}_2\text{O}_6\text{F}]^{5-}$ (dimer), $[\text{Si}_2\text{O}_7]^{6-}$ (dimer), $[\text{SiO}_3\text{F}]^{3-}$ (monomer), $[\text{SiO}_4]^{4-}$ (monomer), which form as a result of addition of structure modifiers [2].

Literature studies show, that there are some conflicting views on the CaF_2 effect on slag structure. Pitch and Tsumaki [3], [4] on the basis of experimental studies have found out that the addition of calcium fluoride causes changes in the silicates structure made of rings and chains. The results were also confirmed with the research by Igouchi [4], [5]. The effect of CaF_2 addition on the structure of silicates is schematically presented in Fig. 1[2]:

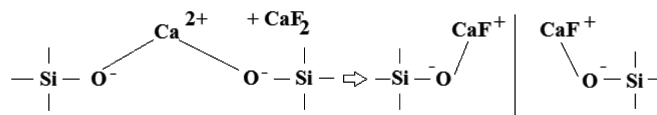
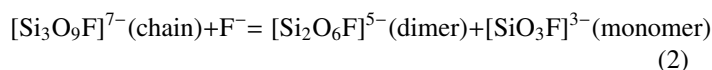
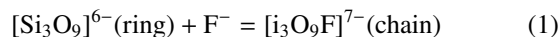
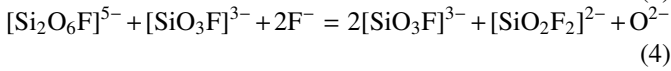
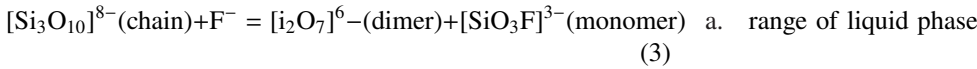


Fig. 1. Effect of CaF_2 addition on the structure of silicates [2]



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Reactions 1 to 4 show the effect of CaF_2 addition on mold slag viscosity. The result of calcium fluoride introduced into slag is depolymerization of the silicate complex and creation of simpler structures. Addition of CaF_2 causes that the reaction will continue to reach simpler silicate slag structure consisting of: dimers: $[\text{Si}_2\text{O}_7]^{6-}$ i $[\text{Si}_2\text{O}_6\text{F}]^{5-}$ and monomer: $[\text{SiO}_3\text{F}]^{3-}$ [6]. Heyeashi [7] observed that the addition of CaF_2 causes polymerization of silicates it by the formation of complex anions CaF^- , this result is a consequence of the presence of Na_2O in the slag. The different behavior of calcium fluoride is due to the chemical composition of the oxide under consideration, mainly the basicity of the slag and the presence of other structure modifiers: Na_2O , K_2O , Li_2O .

Research conducted by [2] confirms that the presence of Na_2O lowers mold slag viscosity. Sodium oxide provides O^{2-} free ions, which react with the bridged O^0 and causes depolymerization of highly crystalline network (Fig. 2)

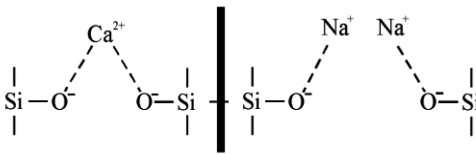
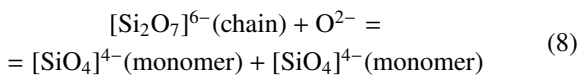
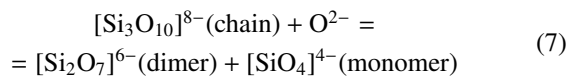
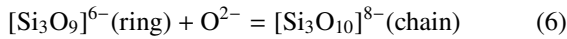


Fig. 2. Effect of Na_2O addition on the structure of silicates [2]

Presence of considerable fraction of Na_2O causes the following changes in the silicates crystal lattice:



Research [2] for the slag $\text{CaO-SiO}_2\text{-Na}_2\text{O}$ with CaF_2 addition shows that the content up to about 8% CaF_2 results in viscosity decrease, while further addition of calcium fluoride has no effect on viscosity reduction. This is also confirmed by simulation calculations mold slags performed by Kalisz [8].

2. Characterization of physicochemical properties of slag

In the literature there are many studies on the system $\text{CaO} - \text{SiO}_2 - \text{Al}_2\text{O}_3 - \text{Na}_2\text{O} - \text{CaF}_2$. The area of liquid phase in the $\text{CaO} - \text{SiO}_2 - \text{Al}_2\text{O}_3$ system at various temperatures can be determined from calculations by means FactSage [9]. Isothermal sections of phase diagram are given in Fig. 3.

a. range of liquid phase

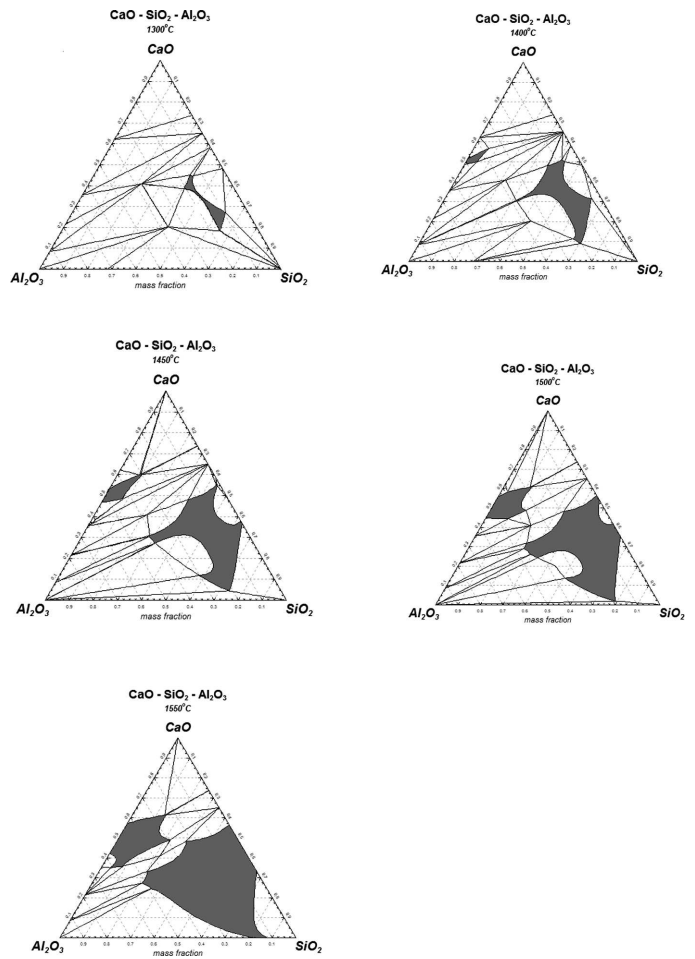


Fig. 3. Region of the liquid phase in the $\text{CaO} - \text{SiO}_2 - \text{Al}_2\text{O}_3$ system at various temperatures, determined from calculations by means of FactSage

b. temperature liquidus

Mold slag is characterized by the temperature liquidus. Melting temperature determines the beginning of solidification and the solidus temperature. There are also softening point, where observed deformation of amorphous solid material of sample. Temperature of softening point is a result of the melting point of the slag components which melt first. Determination of liquidus temperature is possible for a homogeneous sample, previously melted. In the case of powder slag temperature liquidus and solidus are approximate [10].

$$\begin{aligned} T_{\text{liq}}(\text{K}) = &958 + 656, 9\text{XSiO}_2 + 1040, 7\text{XCaO} + 1343, 2\text{XAl}_2\text{O}_3 + \\ &1090, 5\text{XMgO} + 137\text{XNa}_2\text{O} - 668\text{XK}_2\text{O} + 408, 7\text{XLi}_2\text{O} + \\ &522\text{XFeO} + 760, 9\text{XMnO} + 1022\text{XCrO} + 794\text{XFe}_2\text{O}_3 + 2198\text{XCr}_2\text{O}_3 - \\ &532\text{XCaF}_2 + 844\text{XTiO}_2 - 12, 6\text{B}_2\text{O}_3 + 1207\text{XBaO} + 1768\text{XSrO} + \\ &2234\text{XZrO}_2 \end{aligned} \quad (9)$$

c. slag basicity

Basicity index of the slag is the following [11]:

$$B = \frac{2X_{CaO} + 2X_{BaO} + 2X_{CaF_2} + 2X_{Na_2O} - 2X_{Al_2O_3} + 6X_{Fe_2O_3} + (2X_{MgO} + 2X_{MnO})}{X_{SiO_2} + 2X_{Al_2O_3} + X_{TiO_2} + X_{B_2O_3} + (X_{MgO} + X_{MnO})} \quad (10)$$

In the equation we have mole fractions of slag forming oxides. If the MgO content is greater than 7% or MnO content exceeds 4%, the parenthesized expression is in the denominators.

d. viscosity

The viscosity depends on the temperature and chemical composition of the slag, particularly the CaO/SiO₂ contents. SiO₂ – Me_xO quantitative ratio is the rate of polymerization of silicate chains. Me_xO particle causes SiO₄⁴⁻ chain split by compensate for the disrupted electron charge binds to the cation charge. Viscosity ratio was determined with the Nakamoto structural model [12]. The effect of CaF₂ addition was calculated with Urbain model [13].

The Nakamoto model is based on the structure of a liquid solution containing a large amount of oxide SiO₂. The structure consists of SiO₄⁴⁻ ions, that are connected to oxygen “bridged” atoms (O⁰). The presence in the slag-forming metals of I and II groups of the periodic system causes that the silicate chains are disrupted. Oxygen ions O²⁻ located between ions Si⁴⁺ (ion “bridge” O⁰ marked BO) there are arranged at the ends of the chain fragments (ions binding or “non-bridging” O marked NBO). The solution also contain free oxygen ions O²⁻ labelled (FO) from the dissociation of oxides. The effect of Al₂O₃ for modification slag structure depends on the chemical composition of the mold slag.

At low contents of metal oxides of I and II group, Al₂O₃ dissociate into cations Al³⁺ and oxygen anions which break the chains of silicate. However, the share of metal oxides I and II groups is significant, Al₂O₃ creates a tetrahedral structure AlO₃³⁻ like silicate (oxygen ion in this grouping is marked as AlO). Model assumes that the deformation of the structure under the influence of shear stress caused by the velocity gradient, is possible for all four positions of the oxygen ions, but in the case of FO and NBO the susceptibility to deformation is much greater than in the case of BO and AlO.

The dynamic viscosity η dependence of the temperature is given in equation [11]:

$$\eta = A \cdot \exp\left(\frac{E_V}{R \cdot T}\right) \quad (11)$$

where:

E_V – energy activation of viscous flow (J/mol),

$A = 4.80 \cdot 10^{-8}$ (Pa·s),

R – gas constant (J/mol·K),

T – temperature (K).

The model is based on the assumption, that the energy of activation of viscous flow of the E_V is lower if the more the structure of the liquid slag is the places where it is possible to set the network [12]:

$$E_V = \frac{E}{1 + \left(\sum_i \alpha_i \cdot N_{(NBO+FO)} + \sum_j \alpha_{j/Al} \cdot N_{(AlO+BO)} \right)^{\frac{1}{2}}} \quad (12)$$

E is the energy activation for the viscosity of pure SiO₂, defined as: $E = 5.21 \cdot 10^5$ J,

„i” is the index of the components of a liquid solution with the exception of SiO₂,

„j” is the index of the cation (Ca²⁺, Mg²⁺, Fe²⁺, Na⁺, K⁺).

For multi – component system containing SiO₂ and Al₂O₃ and the least two metal oxides of I and II groups:

$$aSiO_2 + \sum b_i (M_x O_y) + cAl_2O_3 = 1 \quad (13)$$

a, b_i, c - number of mole fraction of component

The condition is me for: $a + \sum b_i + c = 1$. If $\sum b_i > c$, than alumina oxide is a structural component of the network. This case is typical of the mold slag. Number of oxygen bonds in tetrahedron Al - O or n (Al-O) attributable to the nature of the cation is:

$$8 \cdot c \cdot \frac{b_i}{\sum b_i} \quad (14)$$

The number of non-oxygen bonds of Si is:

$$2 \cdot b_i - 2 \cdot c \cdot \frac{b_i}{\sum b_i} \quad (15)$$

$$N_{(Al-BO)} = \frac{n_{(O-Al)}}{n_{(SUM-O)}} = \frac{4 \cdot c \cdot \frac{b_i}{\sum b_i}}{2 \cdot a + \sum b_i + 3 \cdot c} \quad (16)$$

$$N_{(NBO-FO)} = \frac{n_{(O-M)}}{n_{(SUM-O)}} = \frac{b_i - c \cdot \frac{b_i}{\sum b_i}}{2 \cdot a + \sum b_i + 3 \cdot c} \quad (17)$$

where:

$N_{(Al-BO)}$ – content of ion “bridge” O⁰,

$N_{(NBO-FO)}$ – content of non-bridging “O marked NBO and free oxygen ions O²⁻ marked (FO) from the dissociation of oxides,

$n_{(SUM-O)}$ – the total number of bonds of oxygen in the system,

$n_{(O-Al)}$ – number of oxygen bonds in the tetrahedron containing the Al,

The parameters for the model calculations are given in Table 1. The parameters were determined by the authors of the model based on the available experimental data for two-, three- and quaternary oxide solutions [12].

TABLE 1

The parameter values for the calculation of the viscosity the oxide solutions by Nakamoto model

$(M_x O_y)_i$	α_i	j	$\alpha_{j/Al}$
CaO	4.00	Ca ²⁺	1.46
MgO	3.43	Mg ²⁺	1.56
FeO	6.05	Fe ²⁺	3.15
Na ₂ O	7.35	Na ⁺	0.27
Al ₂ O ₃	1.14		

The Urbain viscosity model classified the various slag into three categories [13]:

– glass formers:

$$X_G = X_{SiO_2} \quad (18)$$

– network modifier:

$$X_M = X_{CaO} + X_{MgO} + X_{CaF_2} + X_{FeO} + X_{MnO} + X_{CrO} + X_{NiO} + X_{K_2O} + 2X_{TiO_2} + X_{ZrO_2} \quad (19)$$

– amphoteric compounds:

$$X_A = X_{Al_2O_3} + X_{B_2O_3} + X_{Fe_2O_3} + X_{Cr_2O_3} \quad (20)$$

Urbain model makes use of the Weymann equation:

$$\eta = A \cdot T \cdot e^{1000B/T} \quad (21)$$

where:

$$\ln A = -(0.29B + 11.57) \quad (22)$$

The B is calculated by equations:

$$B = B_0 + B_1 X_{SiO_2} + B_2 X_{SiO_2}^2 + B_3 X_{SiO_2}^3 \quad (23)$$

B_0, B_1, B_2, B_3 can be calculated from equation 24-27. These parameters are introduced into equation (23).

$$B_0 = 13.8 + 39.9355\alpha - 44.049\alpha^2 \quad (24)$$

$$B_1 = 30.481 - 117.1505\alpha + 139.9978\alpha^2 \quad (25)$$

$$B_2 = -40.9429 + 234.0486\alpha - 300.04\alpha^2 \quad (26)$$

$$B_3 = 60.7619 - 153.9276\alpha + 211.1616\alpha^2 \quad (27)$$

$$\alpha = \frac{X_M}{X_M + X_A} \quad (28)$$

e. surface tension

Metallurgical slag surface tension is between 0.3 - 0.4 N/m for the acidic slags, and 0.5 - 0.6 N/m for alkaline slags. For binary systems the largest surface tension exhibit systems: MnO - SiO₂, CaO - SiO₂, FeO - SiO₂ and MgO - SiO₂. In this case, the increase of SiO₂ content reduces the surface tension.

For the calculation of the surface tension as a function of solution composition and temperature used in the present work equation Butler as elaborated by Nakamoto et al. [14]. The model assumes that the liquid solution of AX - BY - CZ can be divided into two phases: surface phase and volume phase, which usually differ in chemical composition. Surface phase has a thickness of at most a few molecular layers. The model adopted a unimolecular layer. The Butler equation in Nakamoto [14] version was used to calculate the surface tension as a function of composition and temperature.

$$\sigma = \sigma_{AX}^0 + \frac{R \cdot T}{A_{AX}} \cdot \ln \frac{M_{AX}^{SUR}}{M_{AX}^{VOL}} \quad (29)$$

$$\sigma = \sigma_{BY}^0 + \frac{R \cdot T}{A_{BY}} \cdot \ln \frac{M_{BY}^{SUR}}{M_{BY}^{VOL}} \quad (30)$$

$$\sigma = \sigma_{CZ}^0 + \frac{R \cdot T}{A_{CZ}} \cdot \ln \frac{M_{CZ}^{SUR}}{M_{CZ}^{VOL}} \quad (31)$$

where

indices A, B, are cations and indices X, Y, Z are anions,
 σ – surface tension of solution,

$\sigma_{AX}^0, \sigma_{BY}^0, \sigma_{CZ}^0$ – the surface tension of pure substances AX, BY, CZ,

A_{AX}, A_{BY}, A_{CZ} – surface means for one mole of the substance in the form of unimolecular layer (mono-molecular):

$$A_{AX} = N_0^{\frac{1}{3}} \cdot V_{AX}^{\frac{2}{3}} \quad (32)$$

$$A_{BY} = N_0^{\frac{1}{3}} \cdot V_{BY}^{\frac{2}{3}} \quad (33)$$

$$A_{CZ} = N_0^{\frac{1}{3}} \cdot V_{CZ}^{\frac{2}{3}} \quad (34)$$

where:

N_0 – Avogadro number,

V_{AX}, V_{BY}, V_{CZ} – molar volume AX, BY, CZ,

$M_{AX}^{sur}, M_{AX}^{vol}, M_{BY}^{sur}, M_{BY}^{vol}, M_{CZ}^{sur}, M_{CZ}^{vol}$ – involved substances AX, BY, CZ in the surface and volume phases.

The size of the surface phase is the following:

$$M_{AX}^{sur} = \frac{\frac{R_A}{R_X} \cdot N_{AX}^{sur}}{\frac{R_A}{R_X} \cdot N_{AX}^{sur} + \frac{R_B}{R_Y} \cdot N_{BY}^{sur} + \frac{R_C}{R_Z} \cdot N_{CZ}^{sur}} \quad (35)$$

$$M_{BY}^{sur} = \frac{\frac{R_B}{R_Y} \cdot N_{BY}^{sur}}{\frac{R_A}{R_X} \cdot N_{AX}^{sur} + \frac{R_B}{R_Y} \cdot N_{BY}^{sur} + \frac{R_C}{R_Z} \cdot N_{CZ}^{sur}} \quad (36)$$

$$M_{CZ}^{sur} = \frac{\frac{R_C}{R_Z} \cdot N_{CZ}^{sur}}{\frac{R_A}{R_X} \cdot N_{AX}^{sur} + \frac{R_B}{R_Y} \cdot N_{BY}^{sur} + \frac{R_C}{R_Z} \cdot N_{CZ}^{sur}} \quad (37)$$

The size of the volume phase is the following:

$$M_{AX}^{vol} = \frac{\frac{R_A}{R_X} \cdot N_{AX}^{vol}}{\frac{R_A}{R_X} \cdot N_{AX}^{vol} + \frac{R_B}{R_Y} \cdot N_{BY}^{vol} + \frac{R_C}{R_Z} \cdot N_{CZ}^{vol}} \quad (38)$$

$$M_{BY}^{vol} = \frac{\frac{R_B}{R_Y} \cdot N_{BY}^{vol}}{\frac{R_A}{R_X} \cdot N_{AX}^{vol} + \frac{R_B}{R_Y} \cdot N_{BY}^{vol} + \frac{R_C}{R_Z} \cdot N_{CZ}^{vol}} \quad (39)$$

$$M_{CZ}^{vol} = \frac{\frac{R_C}{R_Z} \cdot N_{CZ}^{vol}}{\frac{R_A}{R_X} \cdot N_{AX}^{vol} + \frac{R_B}{R_Y} \cdot N_{BY}^{vol} + \frac{R_C}{R_Z} \cdot N_{CZ}^{vol}} \quad (40)$$

$R_A, R_B, R_C, R_X, R_Y, R_Z$ – ionic radii of the cations and anions,

$N_{AX}^{sur}, N_{AX}^{vol}, N_{BY}^{sur}, N_{BY}^{vol}, N_{CZ}^{sur}, N_{CZ}^{vol}$ mole fractions of components AX, BY, CZ in the surface and volume phase.

Criterion function is used in the following form:

$$f = (\sigma_{AX} - \sigma_{BY})^2 + (\sigma_{BY} - \sigma_{CZ})^2 + (\sigma_{CZ} - \sigma_{AX})^2 \quad (41)$$

The solution of equation is determined the composition of the surface phase $N_{AX}^{sur}, N_{BY}^{sur}, N_{CZ}^{sur}$ of the values at which the criterion function f reaches the value near zero.

Table 2 contains the ionic radii of the structural components of the slag. Table 3 shows the values for molar volume, which are used for determining the surface area of 1 mole of mono-molecular layers. Table 4 gives the temperature dependence of surface tension for the pure oxides.

TABLE 2
The ionic radii of the structural component of the slag (nm) [14]

Ion	Si ⁴⁺	Al ³⁺	Ca ²⁺	Mn ²⁺	O ²⁻	SiO ₄ ⁴⁻
R [nm]	0.42	0.51	0.99	0.80	1.44	1.86

TABLE 3
Values of molar volume pure components of slag (m³/mol) [14]

Oxide	Values of molar volume pure components of slag (m ³ /mol) dependence on temperature (K)
SiO ₂	$27.516 \{1 + 1 \cdot 10^{-4} (T - 1773)\} \cdot 10^{-6}$
Al ₂ O ₃	$28.3 \{1 + 1 \cdot 10^{-4} (T - 1773)\} \cdot 10^{-6}$
CaO	$20.7 \{1 + 1 \cdot 10^{-4} (T - 1773)\} \cdot 10^{-6}$
MnO	$15.6 \{1 + 1 \cdot 10^{-4} (T - 1773)\} \cdot 10^{-6}$

TABLE 4
The parameters of the model (the dependence of surface tension of pure oxides on the temperature) [14]

Oxide	Correlation between surface tension (mN/m) and temperature (K) for pure oxides	
Al ₂ O ₃	$1024 - 0.177 T$	1473 - 1873 K
CaO	$791 - 0.0935 T$	1573 - 1873 K
MnO	$988 - 0.179 T$	1673 - 1873 K
SiO ₂	$243.2 + 0.031 T$	1673 - 1873 K

3. Object of research

The chemical composition of the slag fed to crystallizer is given in Table 5. This is the original composition, which changes during the process due to the chemical reactions and processes at the steel – slag interfacial region.

TABLE 5
The chemical composition of mold powder i.e. the initial composition of slags

Slag	Chemical composition of powder [% mas.]						
	SiO ₂	CaO	MgO	Al ₂ O ₃	Na ₂ O	Fe ₂ O ₃	CaF ₂
Slag 1	34.4	27.00	3.90	4.70	11.80	1.60	12
Slag 2	34.4	27.00	3.90	4.70	11.80	1.60	0
Slag 3	34.4	27.00	3.90	4.70	11.80	1.60	2
Slag 4	34.4	27.00	3.90	4.70	11.80	1.60	4
Slag 5	34.4	27.00	3.90	4.70	11.80	1.60	6
Slag 6	34.4	27.00	3.90	4.70	11.80	1.60	8
Slag 7	34.4	27.00	3.90	4.70	11.80	1.60	10
Slag 8	34.4	27.00	3.90	4.70	11.80	1.60	14

4. Study of slag viscosity

The coefficients of dynamic viscosity of mold slags were determined with the use of concentric cylinders method. The Fig. 4 presents the schematic of an experimental arrangement.

The graphite crucible of 27 mm internal diameter functioned as the outer cylinder of experimental apparatus. The crucible was placed inside the Tamman furnace. As an internal rotating cylinder the 10 mm graphite rod was applied. The slag samples of the mass 35 g were placed in graphite crucible and heated to 1600°C. The slag1 presented in Table 5 was the subject of experimental investigations. For this

slag composition a series of 10 measurements was carried out. The temperature range under study was 1400 – 1600°C, with 50°C intervals. During the experiments the graphite rod was immersed in molten slag to the depth of 30 mm. The measurements were started at the temperature, at which the slag was completely liquid. This temperature results from the chemical composition, that's why the values for various samples differ considerably. In the measurements the time of one rotation was determined [15]. Table 6 contain the results of the measurement and the calculated values of dynamic viscosity.

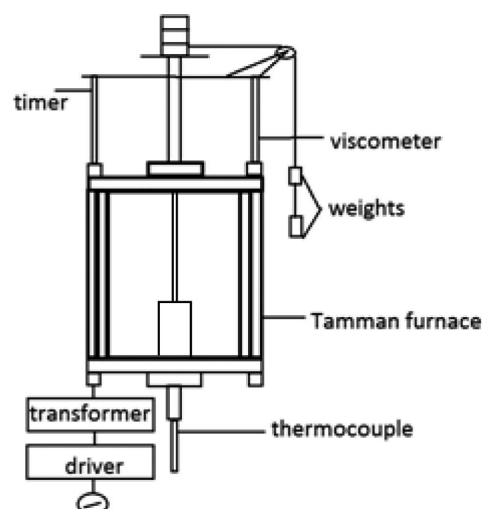


Fig. 4. Schematic view of experimental arrangement for viscosity determination [15]

5. The result of calculation and study

The results of calculations for the viscosity models of Nakamoto and Urbain are shown in Table 6. It was compared with the results of laboratory tests.

TABLE 6
The results of calculations

Model	Temperature [°C]				
	1600	1550	1500	1450	1400
	Viscosity [Pa·s]				
Model Nakamoto Slag 2	0.22	0.33	0.52	0.83	1.374
Model Urbain Slag 2	0.44	0.67	0.93	1.21	1.49
Slag 3	0.41	0.65	0.91	1.18	1.46
Slag 4	0.39	0.62	0.89	1.15	1.43
Slag 5	0.36	0.60	0.85	1.11	1.40
Slag 6	0.34	0.57	0.82	1.109	1.37
Slag 7	0.31	0.55	0.80	1.106	1.34
Slag 1	0.30	0.53	0.77	1.05	1.32
Slag 8	0.28	0.51	0.75	1.02	1.29
Experiment Slag 1	0,10	0,122	0,146	0,170	0,233

Temperature liquidus: 1509°C,
Slag basicity: 1.39.

The results of computer simulations for calculating the surface tension of slag are given in table 7. Calculations were

performed for temperatures 1400, 1500 and 1600°C. Computer simulation was carried out for the CaO – SiO₂ – Al₂O₃ system. Calculations were performed for the surface tension of a solution of 8 configurations where $X_{CaO}/X_{SiO_2} = 1$. Concentration of $X_{Al_2O_3}$ changed in the range of 0.2 – 0.8 and the concentration X_{CaO} and X_{SiO_2} from 0.1 – 0.4. The increase in the content of Al₂O₃ in system causes in an increase of the surface tension of the slag from 471 – 605 mN/m, but increase the concentration of X_{SiO_2} from 0.1 – 0.4 causes a decrease in surface tension. The lowest value of surface tension at a temperature 1600°C, 1500°C and 1400°C were obtained for the following slag composition: $X_{CaO} = 0.4$ and $X_{SiO_2} = 0.4$, $X_{Al_2O_3} = 0.2$, and the highest value for the surface tension of the composition of the slag: $X_{CaO} = 0.1$ and $X_{SiO_2} = 0.1$, $X_{Al_2O_3} = 0.8$.

TABLE 7
The result of surface tension calculation by means of a Nakamoto model

Temperature	Chemical composition of slag [mol fraction]			Surface tension σ [mN/m]
	X_{CaO}	X_{SiO_2}	$X_{Al_2O_3}$	
1600 [°C]	0.4	0.4	0.2	479
	0.35	0.35	0.3	488
	0.3	0.3	0.4	509
	0.25	0.25	0.5	529
	0.2	0.2	0.6	549
	0.15	0.15	0.7	575
	0.1	0.1	0.8	605
1500 [°C]	0.4	0.4	0.2	475
	0.35	0.35	0.3	490
	0.3	0.3	0.4	505
	0.25	0.25	0.5	524
	0.2	0.2	0.6	545
	0.15	0.15	0.7	571
	0.1	0.1	0.8	602
1400 [°C]	0.4	0.4	0.2	471
	0.35	0.35	0.3	484
	0.3	0.3	0.4	500
	0.25	0.25	0.5	519
	0.2	0.2	0.6	540
	0.15	0.15	0.7	566
	0.1	0.1	0.8	598

6. Conclusions

The results obtained from the Nakamoto and Urbain model calculations confirm the effect of temperature and chemical composition on slag viscosity. Urbain model accounts for the influence of CaF₂ additive on the viscosity. This lead to the conclusion that this component of slag reduces the viscosity. Differentiation of the results of model calculations causes from

chemical composition of slag adopted for the calculation. For the calculations performed with the Nakamoto model lower viscosity values were obtained despite the fact that the model does not take into account the additive CaF₂. Assumption was made in the the model Nakamoto, that Al₂O₃ oxide is a component of the structural network taking into account the composition of slag used for calculation was correct. The obtained experimental results at 1400 and 1450°C are an order of magnitude lower than the results of calculations using mathematical models. This indicates that the calculation should also focus on the presence of other constituents of the slag. The reduction process of iron oxides, which occur during the melting of the slag sample during the experiment, should be also taken into account.

Mold slag surface tension is lower than the surface tension of the liquid steel [16]. The surface tension of the slag compound is lower than the surface tension of the pure components constituting the slag. Computer calculations made by the Nakamoto model allow for the assessment of behavior in the mold slag in crystalizer casting machine. These studies are important because the mold slag is involved in the absorption process and the impact of non-metallic inclusions in steel with a layer of solidifying ingot. The behavior of the slag can be assessed on the basis of computer simulation for the ternary system CaO – SiO₂ – Al₂O₃ allows to assess the behavior of the slag, depending on the SiO₂ content and temperature. Addition of SiO₂ reduces the surface tension of the slag, while increasing the content of CaO and Al₂O₃ increases its value[17,18,19].

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