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ASSESSMENT OF SLAG MELT STRUCTURE USING ADAPTIVE SEGMENTED REGRESSION MODEL OF TEMPERATURE-DEPENDENT VISCOSITY AND ELECTRICAL CONDUCTIVITY

Dmytro Stepanenko[1], Nataliya Togobytska[2]

[1]*Z. I. Nekrasov Iron and Steel Institute of NAS of Ukraine, Dnipro, Ukraine*

[2]*University of Applied Sciences (HTW Berlin), Berlin, Germany*

Abstract. *The expediency of using an adaptive segmented regression model for the analysis of logarithmic dependences of viscosity and electrical conductivity on temperature to assess the structure of slag melts is shown. Calculated values of the activation energies of viscosity* (E_η) *and electrical conductivity* (E_χ) *in different temperature ranges. The obtained calculation results confirm that the viscosity and electrical conductivity of slag melts characterize the interaction of various structural particles (ions and/or their groups) and can be used in the study of the structure of slag melts. It was established that the activation energy of viscosity and electrical conductivity decreases as the temperature of slag melts increases. The performed calculations of the indicator* $n = \frac{E_\eta}{E_x}$ *indicate that it can be a criterion for evaluating the structure of the slag melt, when* $n > 1$*, the slag melt is a heterogeneous system, and when* $n < 1$*, it is a homogeneous system. Viscosity and electrical conductivity are interdependent properties and can be predicted if there is data on one of the properties, provided the value of n is known.*

Keywords: *slag, viscosity, electrical conductivity, temperature, structure, adaptive segmented regression model.*

When selecting the optimal composition for slags, viscosity and electrical conductivity stand out as the most informative properties [1–3]. Examination of the fundamental mathematical equations governing the temperature dependency of dynamic viscosity reveals the significant impact of slag structure [4, 5]. Thus, the development of a universal mathematical model for estimating viscosity and electrical conductivity should be based on the "composition-structure-properties" scheme.

There is an empirical dependence according to which electrical conductivity (χ) is related to viscosity (η) as follows [6-8]:

$$\chi^n \cdot \eta = constant. \tag{1}$$

According to Y. I. Frenkel's [6] ideas about the electrical conductivity of ionic melts, particles (ions) are involved in the transfer of electric current, which are able, due to the continuous redistribution of kinetic energy, to pass from one relatively stable state to another. The probability of such displacement under the influence of external field forces is proportional to $e^{-\frac{E_\chi}{RT}}$. It follows from equation (2) that electrical conductivity is a function not only of temperature, but also of the mobility of ions, which significantly depends on the energy of their interaction, which is determined by the chemical composition and is common to both electrical conductivity (E_χ) and viscosity (E_η.).

$$\chi = B \cdot e^{-\frac{E_\chi}{RT}}, \tag{2}$$

$$\eta = A \cdot e^{\frac{E_\eta}{RT}}, \tag{3}$$

The above suggests that electrical conductivity, like viscosity, is determined by the chemical composition of the slag and the structure of its melt. Consequently, it has the capability to reflect phase changes occurring within the melt. Therefore, when studying the viscosity and electrical conductivity of slags as their structurally sensitive properties, it is possible to perform a more detailed assessment of the structural state of melts.

Based on equations (1) - (3), we derive the following

$$\chi^n \cdot \eta = B^n A e^{\frac{-nE_\chi + E_\eta}{RT}}. \tag{4}$$

The product will not depend on temperature, especially if

$$-nE_\chi + E_\eta = 0. \tag{5}$$

From equation (5), it follows that

$$n = \frac{E_\eta}{E_\chi}. \tag{6}$$

For various oxide systems, taking into account the temperature of their melt, the indicator n can be $n > 1$ or $n < 1$, respectively $E_\eta > E_\chi$ and $E_\eta < E_\chi$ [6, 9, 10]. The possibility of inequality $n>1$ and $n <1$ is related to the heterogeneity of aluminosilicate melts. Thus, the inequality $n <1$ is caused by the dissociation of silicon-oxygen anions and the possibility of rearrangement of heteropolar bonds into homeopolar bonds at high temperatures. On the contrary, when $n >1$, the inequality $E_\eta > E_\chi$ is satisfied, which is due to the heteropolarity of bonds between particles in the aluminosilicate melt and its crystallization when the temperature decreases. Therefore, the heterogeneity of slag melts leads to deterioration of diffusion processes in the "metal-slag" system.

Understanding and evaluating these activation energies are essential conditions in studying the fundamental structure of slag melts.

The technique suggested for determining activation energies, as outlined in references [2, 6], relies on utilizing the logarithmic form of equations (2) and (3):

$$\ln(\chi) = -\frac{E_\chi}{R}\left(\frac{1}{T}\right) + \ln(B). \tag{7}$$

$$\ln(\eta) = \frac{E_\eta}{R}\left(\frac{1}{T}\right) + \ln(A). \tag{8}$$

By denoting

$$y = \ln\square(\chi), \qquad x = \frac{1}{T}, \qquad a = \ln(B), \qquad b = -\frac{E_\chi}{R},$$

eq. (1) can be written as

$$y = bx + a. \tag{9}$$

Analogously, equation (8) can be rewritten as (9). If the coeffitients *a*, *b* are known (for example, from experimental data), the activation energies of viscosity (E_η) and electrical conductivity (E_χ) can be calculated using the formula

$$E_\eta, E_\chi = b \cdot R. \tag{10}$$

Hence, this method is based on the construction of piecewise linear relationships between $\ln(\eta, \chi)$ and and its approximation by linear regression in the temperature ranges defined by an expert. However, this identification procedure is notably time-intensive and subject to a degree of subjectivity, impacting the reliability of the estimated activation energies [4]. To address these challenges, we propose a mathematical approach aimed at enhancing the efficiency of this process. In this paper, we use segmented linear regression to calculate activation energies for both temperature-dependent material properties and the temperature values (break points) at which the activation energy changes. Specifically, we use a piecewise linear regression model with unknown breakpoints and number of segments, fitted to experimental data of the electrical conductivity and the viscosity of slag.

Segmented linear regression is widely used in a variety of fields, such as medicine, ecology, and engineering, as published in e.g. [11, 12].The basic idea behind segmented linear regression is to divide the data range into several segments and fit separate linear regression models to each segment. The adaptive aspect of segmented regression refers to the iterative process of identifying the positions of breakpoints. This process involves the global problem of finding estimates for the breakpoint positions and the local problem of fitting line segments given breakpoints.

Using segmented linear regression, the activation energy values of viscosity (E_η) and electrical conductivity (E_χ) were calculated in different temperature ranges ($T_1 \div T_2$) based on experimental data on the viscosity and electrical conductivity of metallurgical slags (the chemical composition of the slag is represented by the basicity indicator CaO/SiO_2) (Table 1). The technique for measuring the viscosity and electrical conductivity of slag melts and some results are described in detail in [1, 4].

Table 1.

Results of calculating the activation energies of viscosity (E_η) and electrical conductivity (E_χ) using segmented linear regression.

CaO/SiO_2	Activation energy of viscosity			Activation energy of electrical conductivity			$n = \frac{E_\eta}{E_\chi}$
	Temperature range (K)		E_η, kJ/mol	Temperature range (K)		E_χ, kJ/mol	
	T_1	T_2		T_1	T_2		
1,109	1872	1651	169,69	1775	1543	175,18	0,97
	1651	1383	245,60	1543	1391	253,16	0,97
	1383	1382	14358,03	1391	1298	414,45	34,64
1,13	1872	1545	178,75	1878	1564	151,65	1,18
	1545	1368	321,95	1564	1396	240,03	1,34
	1368	1367	5394,12	1396	1282	349,60	15,43
1,111	1874	1538	187,81	1873	1660	130,20	1,44
	1538	1368	324,83	1660	1405	230,21	1,41
	1368	1367	11506,74	1405	1286	333,06	34,55
1,235	1874	1610	166,28	1879	1589	149,90	1,11
	1610	1447	258,07	1589	1405	230,71	1,12
	1447	1444	5596,15	1405	1295	342,70	16,33
1,181	1873	1514	184,90	1878	1650	129,37	1,43
	1514	1339	331,98	1650	1412	202,78	1,64
	1339	1324	859,83	1412	1281	323,83	2,66

The obtained results confirm the feasibility of using an adaptive segmented regression model to analyze the logarithmic dependences of viscosity ($\ln(\eta)$) and electrical conductivity ($\ln(\chi)$) on temperature () in order to assess the structure of slag melts on the corresponding segments. The calculated values of activation energies of viscosity (E_η) and electrical conductivity (E_χ) in different temperature ranges ($T_1 \div T_2$) indicate that:

- viscosity and electrical conductivity of slag melts characterize the interaction of various structural particles (ions and/or their groups) and can be used in studying the structure of slag melts;

- with increasing temperature of slag melts, the activation energies of viscosity (E_η) and electrical conductivity (E_χ) decrease;

- the ratio $\frac{E_\eta}{E_\chi} = n$ can be a criterion for assessing the structure of the slag melt. It has been confirmed that when $n > 1$, the slag melt is a heterogeneous system, and when $n < 1$, it is a homogeneous system.

- viscosity and electrical conductivity are interdependent properties and can be predicted if there is data on one of the properties when the n indicator is known.

ОЦІНКА СТРУКТУРИ ШЛАКОВИХ РОЗПЛАВІВ НА ПІДСТАВІ АНАЛІЗУ ТЕМПЕРАТУРНИХ ЗАЛЕЖНОСТЕЙ В’ЯЗКОСТІ ТА ЕЛЕКТРОПРОВІДНОСТІ З ВИКОРИСТАННЯМ АДАПТИВНОЇ СЕГМЕНТНОЇ РЕГРЕСІЙНОЇ МОДЕЛІ

Степаненко Д.[1], Togobytska N.[2],

[1]Інститут чорної металургії ім. З.І. Некрасова НАН України, Дніпро, Україна

[2]University of Applied Sciences (HTW Berlin), Berlin, Germany

Анотація. *Показано доцільність використання адаптивної сегментованої регресійної моделі для аналізу логарифмічних залежностей в’язкості та електропровідності від температури для оцінки структури шлакових розплавів Розраховані значення енергій активації в’язкості (*E_η*) та електропровідності (*E_χ*) в різних діапазонах температур. Отримані результати розрахунку підтверджують, що в'язкість і електропровідність шлакових розплавів характеризуються взаємодію різноманітних структурних частинок (іонів та/або їх груп) і можуть бути використані при дослідженні структури шлакових розплавів. Встановлено, що з підвищенням температури шлакових розплавів зменшуються енергії активації в'язкості і електропровідності. Виконані* *розрахунки показника* $n = \frac{E_\eta}{E_\chi}$ *свідчать про те, що він може бути критерієм оцінки структури шлакового розплаву, при n > 1 шлаковий розплав є гетерогенною системою, а при n < 1 – гомогенною. В'язкість і електропровідність є взаємозалежними властивостями і можуть бути прогнозовані, якщо є дані про одне з властивостей за умови коли відомо значення n.*

Ключові слова: *шлак, в’язкість, електропровідність, температура, структура, адаптивна сегментована регресійна модель.*

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