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APPLICATION OF THE IIDA MODEL FOR ESTIMATION OF SLAG VISCOSITY FOR Al_2O_3-Cr_2O_3-CaO-CaF_2 SYSTEMS

ZASTOSOWANIE MODELU IIDA DO OBLICZANIA LEPKOŚCI ŻUŻLI Al_2O_3-Cr_2O_3-CaO-CaF_2

The half-empirical model of Iida was applied for estimation of slag viscosities for Al_2O_3-Cr_2O_3-CaO-CaF_2 systems. The model is based on a hypothetical viscosity of a slag being a sum of viscosities of the components and the slag basicity index which is modified respectively. The model uses two temperature-dependent parameters which are fitted for each group of the slags on the base of experimental viscosity data. The slags considered in this work were composed of ca. 5% Cr_2O_3, 17-28%CaO, while % Al_2O_3 was dependent on %CaO, i.e., the %Al_2O_3/%CaO ratio was within 2.0 to 3.4 by %CaF_2 up to 10%. Applicability of the Iida model for these slags was evaluated in two ways: (i) based on the typical slag basicity index, *B* and (ii) the optical basicity, Λ. Basing on experimental viscosity data for the slags for a 1873-1993K temperature range, the temperature parameters were established. For the case of the slags with no CaF_2, a satisfactory aggreement between a semi-empirical formula and the experimental data was found, yet the parameters' fitting was superior when the slag basicity index *B* was applied instead of the optical basicity, Λ. For the slags containing CaF_2, in which viscosity distinctly goes down with increasing %CaF_2, neither B nor Λ – computed from typically applied relationships – gave acceptable estimates of the viscosity. Therefore, the both indices are to be substituted by the modified ones, which – despite of the fact that they have some hidden physical meaning – are to be considered rather as model fitting parameters. The performed computations point out that the model of Iida is a convenient and a relatively simple tool for viscosity estimates, yet only within a particular group of slags.

Keywords: slag viscosity, Iida model, basicity index, optical basicity

W pracy zastosowano półempiryczny model lepkości Iida do ciekłych żużli Al_2O_3-Cr_2O_3-CaO-CaF_2. Model ten opiera się na hipotetycznej lepkości żużla będącej sumą lepkości składników oraz na wskaźniku zasadowości żużli, który jest odpowiednio zmodyfikowany. Model zawiera dwa parametry będące funkcją temperatury, które są dopasowywane, dla danej klasy żużli, na podstawie eksperymentalnych wartości lepkości. Rozważane w pracy żużle miały po ok. 5% Cr_2O_3, 17-28%CaO, % Al_2O_3 zależny był od %CaO, tzn. stosunek %Al_2O_3/%CaO był równy od 2,0 do 3,4, %CaF_2 był równy od 0 do 10%. Porównano przydatność modelu Iida do tych żużli przeprowadzając dwa warianty obliczeń – w oparciu o typowy wskaźnik zasadowości *B* oraz zasadowość optyczną Λ. W oparciu o znane eksperymentalne wartości lepkości tych żużli w zakresie 1873-1993K dobrano parametry temperaturowe w równaniu Iida. W przypadku żużli bez CaF_2 uzyskano dobrą zgodność półempirycznego równania z danymi eksperymentalnymi, jednak dopasowanie parametrów w przypadku wskaźnika zasadowości *B* okazało się bardziej efektywne niż w przypadku zasadowości optycznej Λ. Dla żużli zawierających CaF_2, w których lepkość znacznie spada ze wzrostem %CaF_2, ani wskaźnik *B* ani Λ, obliczany wg ogólnie stosowanych zależności, nie daje poprawnego opisu lepkości. Konieczne jest zastąpienie ich przez wartości zmodyfikowane, które, choć mają ukryty sens fizyczny, należy raczej traktować jako parametr modelowy. Obliczenia wykazują, że model Iida jest wygodnym i w miarę prostym modelem do obliczania lepkości, lecz tylko w obrębie danej klasy żużli.

1. Introduction

There are usually two ways when looking for the appropriate formulae for estimation of the viscosity parameter of slags as a function of composition and temperature. One may, for instance, define the structural factor of the slag, then - basing on experimental viscosity data for different temperatures – the temperature parameters are matched. Thus obtained equations are of a semi-empirical type. They can be applied only to a particular group of slags due to the interdependence of the temperature parameter – fitted on the base of experimental viscosity data – and the assumed structural factor. It is no doubt a substantial drawback of the model while some assets consist in the apparent form of the model equation which makes its application easier. One of the

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models leading to semi-empirical form is the model of Iida [1,2].

The other way is a step-wise procedure specific in beginning with two-component slags then coming to more component ones , e.g.., slag viscosity of a ternary A-B-C is computed on the base of the measured binaries as follows: A-B, A-C, B-C. The operation needs some complex computation as well as the knowledge of thermodynamic data for slag components. It is applied by commercial computer programs.

In this study it will be attempted to apply the Iida model to a particular group of slags.

2. Model of Iida

According to Iida the slag viscosity may be given by the formulae [1,2]

$$\mu = a(T) \cdot \mu_0 \cdot \exp(b(T)/B) \qquad (1)$$

which contains the slag basicity index B, substituted typically by a modified index B^* (fitting parameter), the theoretically calculated viscosity of a hypothetic slag μ_0 and the parameters $a(T)$, $b(T)$ established from empirical data by fitting technique. Index B^* is the corrected quantity of B, assumed for a selected group of slags.

The viscosity μ_0 corresponds to the one which would have an oxide solution (slag) for the case when their components do not form any special structures. It is set as an additive sum of hypothetic viscosities of the components multiplied by their mole ratios:

$$\mu_0 = \sum_{i=1}^{n} \mu_{0i} X_i, \qquad (2)$$

where n – the number of the slag components, X_i – the components' mole ratios, μ_{0i} – the hypothetic viscosities of the components.

The hypothetic viscosities of the components μ_{0i} are computed from [1] as follows:

$$\mu_{0i} = 1.8 \cdot 10^7 \cdot \frac{(M_i \cdot T_{mi})^{1/2} \cdot \exp(H_i/RT)}{V_{mi}^{2/3} \cdot \exp(H_i/RT_{mi})} \quad [\{\mathrm{Pa \cdot s}\}], \qquad (3)$$

where M_i – mole mass [kg/mole], T_{mi} – melting temperature [K], V_{mi} – mole volume [m^3/mol], H_i – melting enthalpy [J/mole] of individual components "i".
H_i is computed from a simplified formula [1]

$$H_i = 5.1 \cdot T_{mi}^{1.2} \quad [\mathrm{J/mol}]. \qquad (4)$$

Formula (1) requires a theoretical computation of the hypothetic viscosity μ_0, which is a function of the slag's composition and temperature, then the basicity index B or taking of the assumption with regard to its modification into B^* (dependent of the type of the slag), and finally, establishing the parameters $a(T)$ and $b(T)$ by fitting technique to make them adequate for a given temperature range and for a definite group of slags.

3. Application of the Iida model

3.1. Characteristics of the slags used for computations

The model of Iida was applied for the slags composed of Al_2O_3-CaO-Cr_2O_3-SiO_2-MgO-Na_2O-FeO-CaF_2, for which the experimental viscosity data were known for the temperatures of 1873, 1893, 1923, 1938, 1973 and 1993K [3]. The slags were divided into the groups specific in the constant Al_2O_3/CaO mass ratios equal to: 2.0; 2.5; 3.0 and 3.4. Within each group, the CaF_2 content was respectively: 0; 4; 10% mass. All of them contained about 5 % Cr_2O_3 each with small contents of MgO, Na_2O, SiO_2 and FeO. In Tab.1 are set the chemical compositions of the selected slags.

TABLE 1

The chemical compositions of the slags, in % mass (they are numerated according to [3])

%SiO_2	%Al_2O_3	%CaO	%MgO	%Na_2O	%Cr_2O_3	%FeO	%CaF_2	Slag No.	$\frac{\%Al_2O_3}{\%CaO}$
1.85	57.36	28.64	2.15	4.58	4.12	1.3	0	1	2
1.95	54.18	27.1	2.34	4.85	4.15	1.43	4	3	2
1.95	50	25	2.33	4.82	4.18	1.72	10	6	2
3	58	23	2	6	5	3	0	7	2.5
2.88	55.77	22.12	1.9	5.75	4.7	2.88	4	9	2.5
2.45	52.75	21.1	1.9	4.95	4.9	1.95	10	12	2.5
3.5	60	20	2.5	5	5.5	3.5	0	13	3
3.36	57.69	19.23	2.4	4.75	5.2	3.36	4	15	3
2.39	54.9	18.3	2.31	4.62	5.1	2.39	10	18	3
3.4	62	18.23	2.5	4.9	5.4	3.4	0	19	3.4
3.32	59.6	17.52	2.4	4.6	5.2	3.36	4	21	3.4
3.08	56.36	16.57	2.27	3.7	4.87	3.15	10	24	3.4

3.2. Computation of a hypothetic slag viscosity μ_0, the basicity index B and the optical basicity Λ

In Tab.2 there are presented the data set for individual slag components used in this study and the μ_{0i} ones computed from them at temp. 1873K.

TABLE 2

T_{mi}, V_{mi}, α_i and Λ_i used for calculations together with the computed H_i and the viscosities μ_{0i} of the slag components at 1873K

Component	T_{mi} [K]	V_{mi} [10^{-6} m^3/mole]	H_i [J/mole]	μ_{0i} at 1873K [10^{-3} Pa · s]	α_i	Λ_i
SiO_2	1993	8.2	46449	2.54	1.48	0.48
Al_2O_3	2320	33.3	55739	5.33	0.10	0.60
CaO	2860	21.1	71649	14.6	1.53	1.0
MgO	3073	22.9	78099	17.6	1.51	0.78
Na_2O	1193	33.5	25092	0.59	1.94	1.15
FeO	1641	15.6	36788	2.4	0.96	1.0
CaF_2	1691	31.01	38137	1.61	1.53	0.43
Cr_2O_3	2573	38	63110	9.49	0.13	0.7

The data of "hypothetic viscosity" of the slags – computed on the base of the data of Tab.2 – for the temperature 1873K are presented in Tab.3.

The Iida model will be deployed in the original variant, i.e., for the index B and the optical basicity Λ.

The basicity index B was computed using the formulae generally applied as:

$$B = \frac{\sum_i \alpha_i \cdot \%mas.i}{\alpha_{SiO_2} \cdot \%mas.SiO_2 + \alpha_{Al_2O_3} \cdot \%mas.Al_2O_3}, \quad (5)$$

where α_i for the components are presented in Tab.2.

By another variant, the optical basicity Λ was computed from the formula:

$$\Lambda = \frac{\sum_i \Lambda_i \cdot n_i \cdot X_i}{\sum_i n_i \cdot X_i}, \quad (6)$$

where X_i is the mole ratio, n_i – a number of oxygen atoms of the molecule (equal to 2 for CaF_2). The basicities Λ_i for individual components are presented in Tab.2.
The B and Λ data for the investigated slags are set in Tab.3.

TABLE 3

The basicity index B and the optical basicity Λ for the investigated slags and the hypothetic viscosities μ_0 at temp.1873K

Slag No.	B	Λ	μ_0 at 1873K [mPa · s]
1	6.813	0.7051	9.26
3	7.519	0.6952	8.92
6	8.701	0.6793	8.41
7	5.213	0.6954	8.39
9	5.830	0.6845	8.12
12	7.029	0.6669	7.86
13	4.307	0.6836	8.20
15	4.867	0.6731	7.93
18	6.503	0.6592	7.63
19	4.019	0.6776	8.01
21	4.541	0.6674	7.74
24	5.387	0.6508	7.41

3.3. Setting the temperature coefficients a(T), b (T) for slags with no CaF_2

On the base of the experimental viscosity data μ_{exp} for the slags with no CaF_2 (slags No. 1, 7, 13, 19 – in Tab.1) and the computed μ_0 data, there were plotted the followings: $[\ln(\mu_{exp}) - \ln(\mu_0)]$ as a function of $1/B$ index and of $1/\Lambda$ for the temperatures 1923, 1938, 1973 and 1993K (for temp. 1873 and 1893K the data for the slags are lacking, i.e., for the all range of B and Λ data):

$$\ln(\mu_{exp}) - \ln(\mu_0) = \ln[a(T)] + b(T)/B \quad (7)$$

$$\ln(\mu_{exp}) - \ln(\mu_0) = \ln[a(T)] + b(T)/\Lambda \quad (8)$$

As the index B or Λ defined as such do not depend on temperature, thus for a constant temperature, the plots ought to be of a linear character. The results are presented in Fig.1 for B and in Fig.2 for Λ. Using the obtained data for a and b for particular temperatures there were found the temperature relationships $a(T)$ and $b(T)$. The results are presented in Fig.3 for $a(T)$ and in Fig. 4 for $b(T)$. They were used for the subsequent computations applying the equations below:
for B

$$a(T) = 242,4 - 0,1021 \cdot T \quad (9)$$

$$b(T) = 299,8 - 0,2946 \cdot T + 7,313 \cdot 10^{-5}T^2 \quad (10)$$

for Λ

$$a(T) = -0,5127 + 2,713 \cdot 10^{-4}T \quad (11)$$

$$b(T) = 467,8 - 0,4579.T + 1,1334 \cdot 10^{-4}T^2 \quad (12)$$

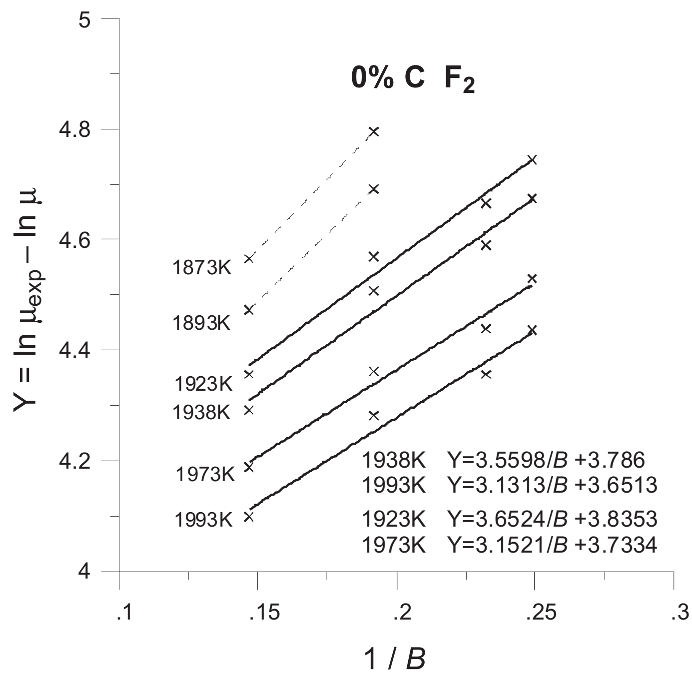

Fig. 1. The linear relationship between ($\ln\mu_{exp}$ - $ln\mu_0$) and reciprocal basicity index, $1/B$, for slags with no CaF_2 content, for temperatures 1923, 1938, 1973 and 1993K

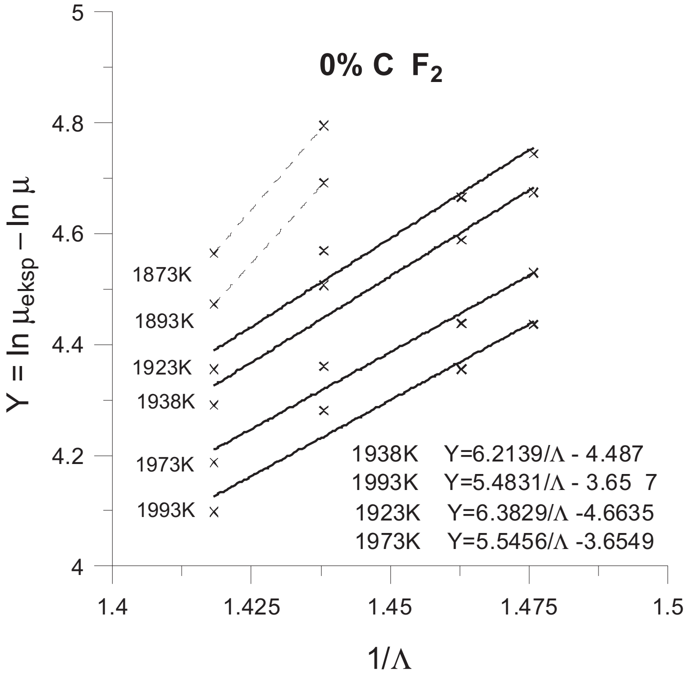

Fig. 2. The linear relationship between ($\ln\mu_{exp}$ - $ln\mu_0$) and reciprocal optical basicity, 1/Λ, for slags with no CaF_2 content, for temperatures 1923, 1938, 1973 and 1993K

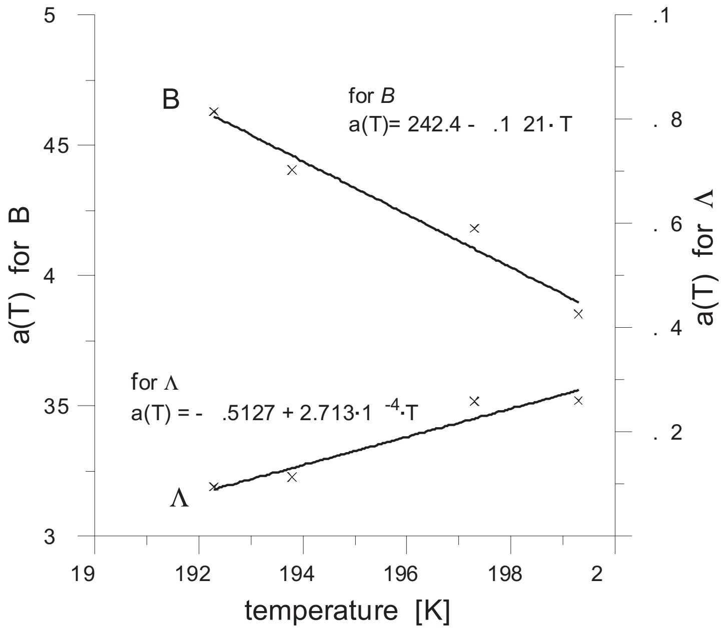

Fig. 3. The temperature relationship $a(T)$ for the model based on the basicity index, B, and the optical basicity Λ

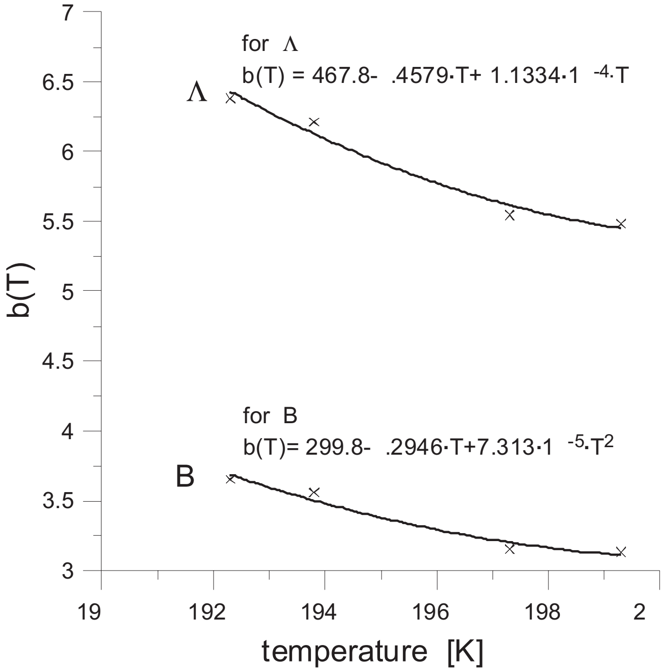

Fig. 4. The temperature relationship $b(T)$ for the model based on the basicity index, B, and the optical basicity Λ

The computed viscosity data were compared to the experimental ones for the slags with no CaF_2. The results are presented in Fig.5 for B and in Fig.6. for Λ. For the case of the basicity B a fairly good agreement was found for the entire temperature range, while for Λ the discrepancies are higher. It is due to the fact that the range of B is extensive, which makes fitting the parameters a and b easier, contrary to Λ.

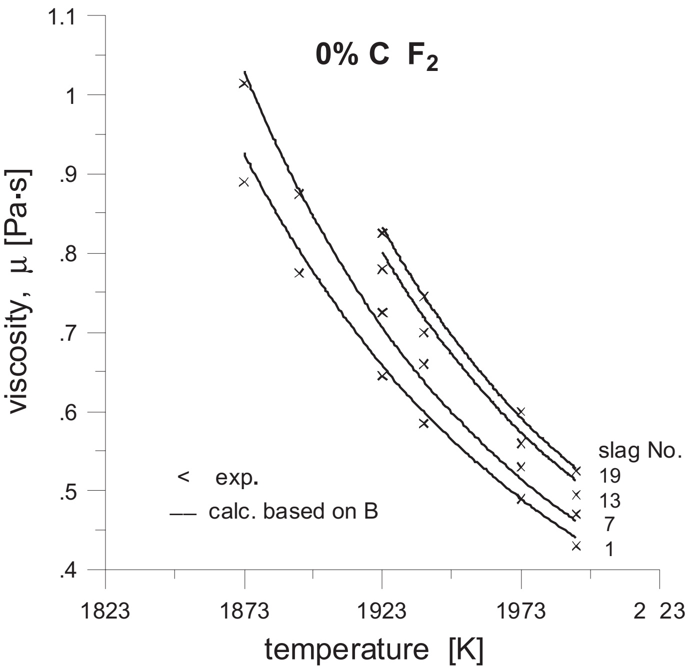

Fig. 5. The comparison of the computed viscosities based on the basicity index, B, with the experimental data for the slags with no CaF_2

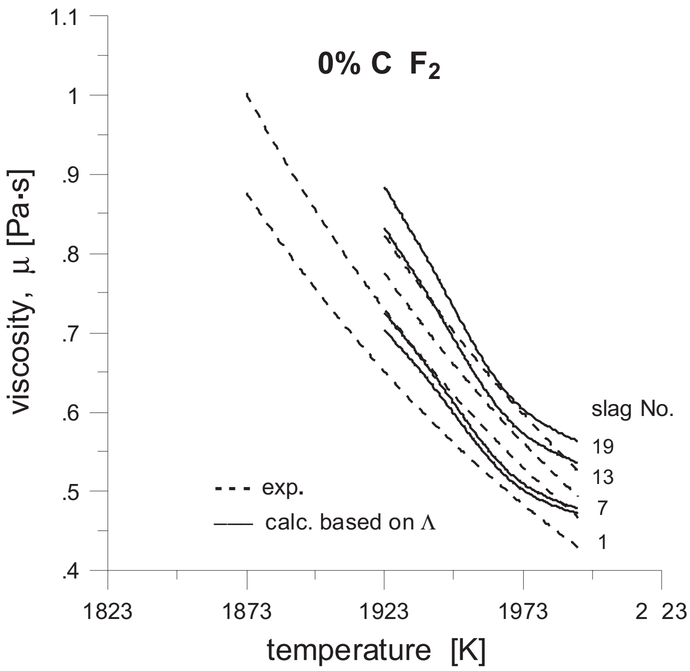

Fig. 6. The comparison of the computed viscosities based on the optical basicity index, Λ, with the experimental data for the slags with no CaF_2

3.4. Slags with a high CaF_2 content

For the slags of a high content of CaF_2, the viscosities drastically go down. Simultaneously *B* and Λ are getting changed, but in opposite direction, i.e., *B* goes up substantially which enhances the viscosity drop, while Λ slightly goes down. Therefore, it gets possible some correction of *B* in order to make its increase bigger. For the Λ case, it would be necessary to inverse the direction of the changes by increasing CaF_2 content. Thus, the index *B* seems to be more apt for the model of Iida.

On the base of the parameters *a* and *b* fitted to the slags with no CaF_2, it was assumed that they would be appropriate for the slags with CaF_2 and basing on them the index *B* was corrected and it was considered as the one dependent on the preliminary *B* and CaF_2 content. The conversion factor used for that correction became in fact the third fitting parameter of the model of Iida. It is to note that also the model's author Iida considers the index *B* in the same way. However, this procedure makes it difficult to find a precise, theoretical justification for the correction, so the all fitting model Iida parameters obey only within some definite group of slags. For the analysis of the behaviour of *B* by increasing $\%CaF_2$, there was assumed the following correction of that index:

$$B_{corr} = B \cdot [0,033 \cdot (\%\mathrm{CaF_2})^2 + 0.17 \cdot \%\mathrm{CaF_2} + 1] \quad (13)$$

which obeys for the slags with $\%Al_2O_3/\%CaO>2$ (apart from the slags No.3 and 6 which have got the lowest viscosity).

In Fig. 7, 8 and 9 are compared the computed data for viscosity to the experimental ones, they agree fairly well.

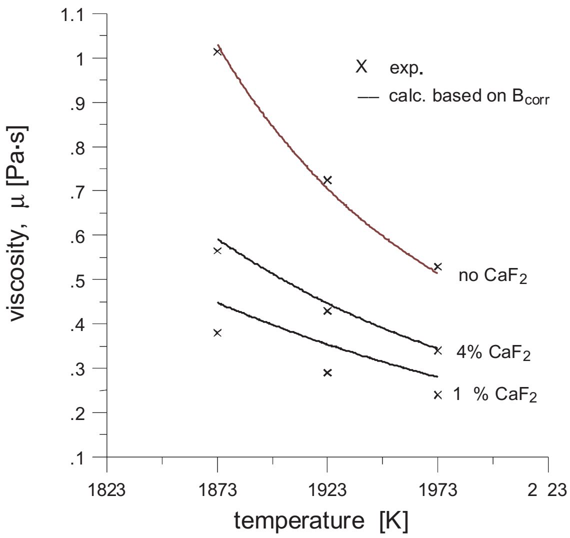

Fig. 7. The comparison of the computed viscosities by using the corrected basicity index, B_{corr}, as a model fitting parameter, with the experimental data for the slags No.7, 9 and 12 of different contents of CaF_2 and the constant Al_2O_3/CaO mass ratio equal to 2.5

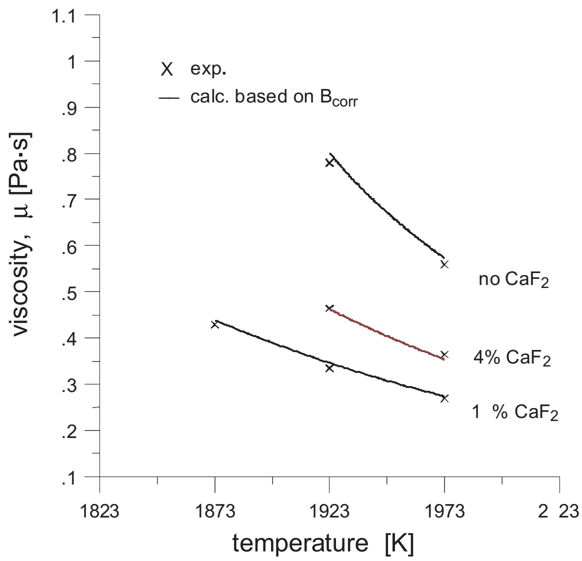

Fig. 8. The comparison of the computed viscosities by using the corrected basicity index, B_{corr}, as a model fitting parameter, with the experimental data for the slags No.13, 15 and 18 of different contents of CaF_2 and the constant Al_2O_3/CaO mass ratio equal to 3

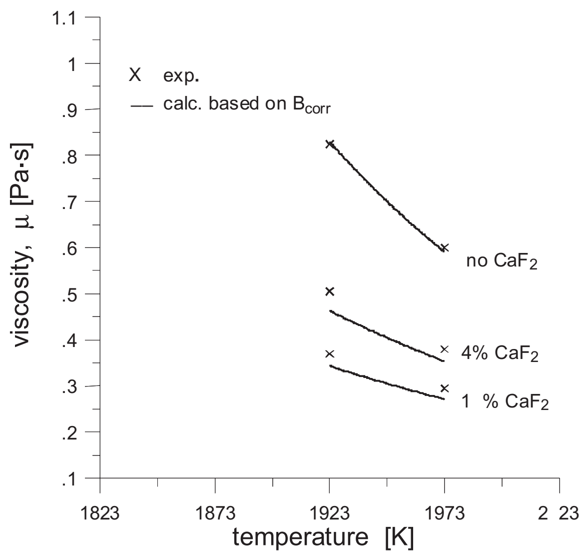

Fig. 9. The comparison of the computed viscosities by using the corrected basicity index, B_{corr}, as a model fitting parameter, with the experimental data for the slags No.19, 21 and 24 of different contents of CaF_2 and the constant Al_2O_3/CaO mass ratio equal to 3.4

4. Conclusions

The performed by the authors analysis of the applicability of the model of Iida to some group of slags indicates that for the considered slags it is possible to model them by using either the index *B* or the optical basicity index Λ, on the condition the slags do not contain calcium fluoride. It was found that the index *B* was more useful for the model computations.

The presence of CaF_2 in a slag decreases its viscosity so strongly, that the change of *B*, effected by CaF_2 presence, which results from generally applied formulae, is not sufficient. Therefore, some substantial correction of that index is required before it is applied for the Iida model equation.

The optical basicity Λ requires a significantly more extensive correction as the direction of the changes must be reversed, i.e., generating an increase and not a decrease by increasing CaF_2 content.

The performed analysis of applicability of the model of Iida for the investigated slags indicates that the model – which is relatively simple – may be conveniently used but its parameters must be every time adjusted for a definite group of slags.

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