

**APPLICATION OF COMPUTATIONAL MODEL
FOR ALUMINA DISSOLUTION IN MOLTEN SLAG**
**ỨNG DỤNG MÔ HÌNH TÍNH TOÁN QUÁ TRÌNH HÒA TAN ÔXYT NHÔM
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ABSTRACT

This paper presents application of a computational model for the dissolution of alumina inclusion in molten slag for steelmaking. The slag systems used in the present research was similar to those containing CaO-SiO₂-Al₂O₃ which have applications in practice. The model was counted on some assumptions such as inclusion was initially 100% of alumina, activity was equal to concentration (in wt%) everywhere in the domain and alumina diffusion in the liquid slag was the rate-limiting step of the dissolution. The dissolution rates of alumina calculated from the model results were compared with other experimental results. It is certain that this model can be used for computation involving alumina dissolution in molten slag during steelmaking process.

TÓM TẮT

Bài báo trình bày kết quả ứng dụng mô hình tính toán quá trình hòa tan tạp chất ôxyt nhôm trong xỉ nóng chảy khi luyện thép. Xi sử dụng trong nghiên cứu này là hệ 3 nguyên CaO-SiO₂-Al₂O₃ tương tự như trong thực tế. Mô hình tính toán được xây dựng với giả thiết tạp chất ban đầu chứa 100% ôxyt nhôm, hoạt độ của các cấu tử là nồng độ (tính theo % khối lượng) ở mọi vị trí tính toán và sự khuếch tán của ôxyt nhôm trong xỉ lỏng là khâu quyết định tốc độ của quá trình hòa tan. Tốc độ hòa tan của ôxyt nhôm trong xỉ lỏng được xác định dựa trên kết quả chạy mô hình và so sánh với các nghiên cứu thí nghiệm khác. Kết quả cho thấy mô hình này có thể sử dụng cho các bài toán liên quan đến sự hòa tan tạp chất ôxyt nhôm vào xỉ lỏng trong luyện thép.

I. INTRODUCTION

Modern technology makes increasingly stringent requirements for materials working in conditions of high pressures, velocities, deformation, aggressive environments [1]. In steelmaking, the concept “clean steel” refers to very low content of harmful inclusions because non-metallic inclusions as alumina degrade the mechanical properties and thereby lower the ductility of the final products. Therefore, the solid inclusions must be removed by dissolving in slag phase covering the liquid steel in the ladle, tundish or mold during production [2÷4]. It is usually expected that rapid dissolution of these inclusions in the molten slag can be obtained to prevent the entrapment by the liquid steel. In this case, the quality of liquid steel becomes worse; and it sometimes causes several failures for continuous casting [5]. Many experimental works have been done so far to determine dissolution rate of alumina in molten slag [6÷8]. It was concluded that the dissolution rate is influenced by many factors, e.g. slag compositions, temperature, convection

flow and so on. However, the experiment on such topic proves to be difficult, expensive and time consuming. In such situations, computational model offers reliable results if using a proper solution.

The focus of this paper is on the computational model of alumina dissolution in a given CaO-SiO₂-Al₂O₃ slag system. The predicted rate was compared with the experimental data of the other researches to consolidate the validation of the used model.

II. THE COMPUTATIONAL MODEL

2.1. Conditions for application

When an alumina inclusion is in contact with the molten slag, it gradually liquefies through the formation of liquid boundary layer at the interface then dissolves completely after a certain time. As mentioned in the reported findings [6÷8], alumina diffusion in the liquid CaO-SiO₂-Al₂O₃ slag is considered as the rate-limiting step for the alumina dissolution process. Thus, the concentration profile of CaO and Al₂O₃ must be similar as illustrated in Fig.1

different extension. The program then proceeds to produce output. The output may be a movie file (.avi) or text files (.out) as demanded by user. An example of the input file for running the present model is shown in Fig. 3, in which the value of diffusion coefficients at 1550°C is selected according to the references [6,8÷10]. The fact that alumina diffusion in liquid slag is dependent on the chemical composition [2,8] suggests that the value of diffusion coefficients must be changed for each computed slag. It suggests that the diffusion

III. RESULTS AND DISCUSSION

Chemical composition of the slag used to compute is listed in Table 1. These slags were employed in the research works performed by Junhu Liu *et al.* [6] and A. H. Bui *et al.* [8], in whose experiments, the dissolution rate (in mm·s⁻¹) of alumina inclusion in molten slag was determined by decrease of the immersed particle radius with time [6] or by erosion thickness of the dipped rotating alumina rod with time [8]. In this study, the predicted rate (in mm·s⁻¹) was estimated using the following equation, Eq. (1):

$$R_d = \frac{d}{t} \dots\dots\dots (1)$$

where *d* (mm) is the movement distance of the liquid slag/solid inclusion interface during the modeling time *t* (s).

Table 1. Chemical composition of the computed slag (in wt%).

Slag	CaO	SiO ₂	Al ₂ O ₃
[6] A	29.7	46.2	24.1
[8] B	48.7	46.3	4.99
C	43.5	41.5	14.9
D	38.4	36.7	24.9

Since the difference in the slag composition was considered, diffusion coefficients in the liquid bulk slag (D1) and in liquid boundary layer (D2) were valued as presented in Table 2. Meanwhile, the value of solid alumina diffusion coefficient (D3) has been kept as constant as 10⁻⁹ mm²·s⁻¹ according to A.O. Araromi [9] for running the computational model. Acknowledging that the

diffusion in the case where alumina rod rotates in the molten slag has an advantage compared to that in the case where alumina particle immerses in the molten slag, the D2 value for the first must be larger than that for the latter. This means that D2 was 3.5×10⁻⁵ mm²·s⁻¹ for slag A [6], but was selected as 5×10⁻⁴ mm²·s⁻¹ for the rest slags in this study based on the reported findings [8÷10]. The values of D1 were taken according to A. H. Bui *et al.* [8]. In practical, some oxides such as Na₂O, K₂O, B₂O₃, CaF₂, etc are usually added in the CaO-SiO₂-Al₂O₃ slag system. The introduction of the above modifying additives to the slag results in substantial change in the slag viscosity, the incipient crystallization temperature and dissolution rate of the oxide inclusions.

Table 2. The selected diffusivity coefficients at 1550°C for modeling (in mm²·s⁻¹).

Slag	D1	D2	D3
[6] A	6.0×10 ⁻⁶	3.5×10 ⁻⁵	10 ⁻⁹
[8] B	7.5×10 ⁻⁶	5.0×10 ⁻⁴	10 ⁻⁹
C	7.0×10 ⁻⁶	5.0×10 ⁻⁴	10 ⁻⁹
D	6.0×10 ⁻⁶	5.0×10 ⁻⁴	10 ⁻⁹

A typical concentration profile for modeling the alumina dissolution in the above slags is illustrated in Fig. 4. It is clear that the liquid slag/solid inclusion interface moved to the right side during the simulated time, the liquid boundary layer was formed as soon as the modeling started and then its thickness increased with the simulated time. Fig. 4 shows that the alumina concentration in the liquid slag was constant as zero as assumed because amount of the dissolved alumina was very small compared to the bulk volume. This is in consistent with the condition of experiments [4,6,8]. Since the diffusivity coefficient of alumina in the liquid slag was smaller than that in the liquid boundary layer (see Table 2), it required a longer distance for the alumina concentration to reach the value of the bulk. Obviously, the higher value can make the mass transport easier and consequently shorten this distance. coefficients must be chosen very carefully.

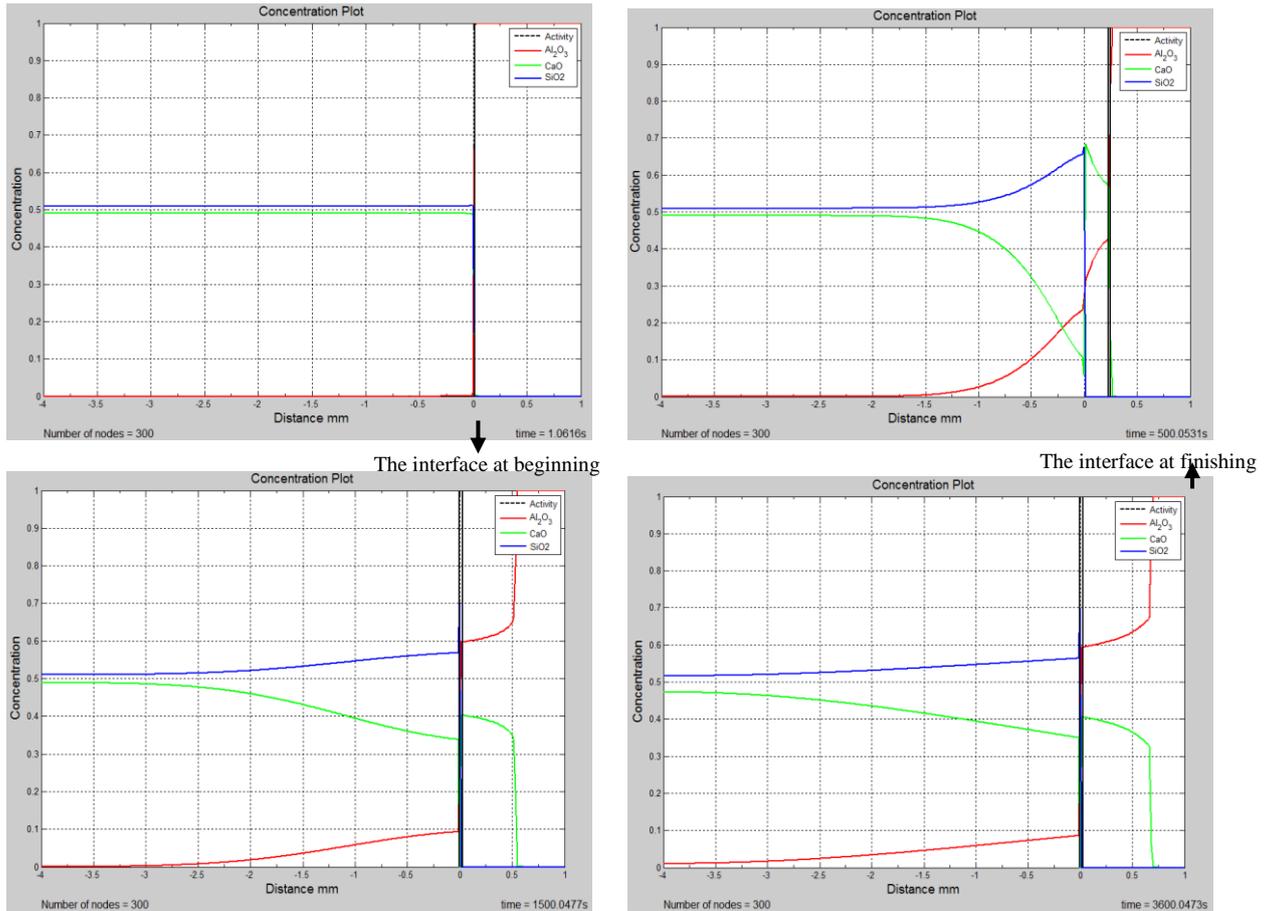


Fig. 4 Change in the concentration profile during modeling (for slag B).

By taking the dissolved thickness and the modeling time into account, the average dissolution rate of alumina in the molten slag can be estimated. In order to ensure the same dissolved time with the experimental, the rates were calculated after 2000s modeling for slag A and 3600s modeling for the rest slag. The obtained rates were compared with the experimental and shown in Table 3. The fact that a good agreement was met for slag containing 5~15% Al_2O_3 (B and C) while a difference was occurred for slag containing about 25% Al_2O_3 (A and D) between the predicted and the experiment rates indicates that this model could be applied for the slag system which had not contained a high alumina concentration. This can be explained that a high alumina concentration of the slag caused a decrease in the concentration driving force, a factor affecting the dissolution rate of alumina [8]. This must be studied deeply to modify the

mathematical algorithms of this model so that it can be compute for dissolution of other oxide inclusions in many types of the molten slags.

Table 3. Comparison of the Al_2O_3 dissolution rates at $1550^\circ C$.

	Modeling ($mm \cdot s^{-1}$)	Experimental ($mm \cdot s^{-1}$)
Slag A	0.00042	0.00012
Slag B	0.00018	0.00012
Slag C	0.00015	0.00009
Slag D	0.00033	0.00006

IV. CONCLUSIONS

A study on alumina dissolution in the molten $CaO-SiO_2-Al_2O_3$ slags was done using a computational model. The dissolution rates calculated from the modeling results were compared with other experimental data. It is concluded that the validation of the

computational model was confirmed through a good agreement between the predicted and experimental rates. However, selection of suitable diffusion coefficients is very important to achieve more precise modeling results. It is suggested that this computational model is applicable to design a slag, in which alumina inclusions can be dissolved quickly. Further works should be concerned and carried out in

order to employ the modified model for other oxide inclusions in steelmaking industry.

Acknowledgment

A part of this research was done in the Metals Processing Simulation Lab (UIUC) during the author's training time under the financial support of The Advanced Program in Materials Science and Engineering (HUT).

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