ESTIMATION OF PHYSICAL PROPERTIES OF MOLTEN MOLD FLUX BY NEURAL NETWORK COMPUTATION

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ABSTRACT

Physical properties of mold flux, such as viscosity and surface tension, are very important factors for the control of various phenomena in a continuous casting mold. Although accurate evaluation of physical properties is required, it is quite difficult to find adequate data to apply directly to each mold flux with complex compositions. Thus, some estimation models based on physico-chemical theory have been proposed so far, but there is no adequate model to estimate the physical properties for wide temperature and composition ranges in any kinds of multi-component mold fluxes.

Neural network computation is one of numerical estimation methods to cope with the above problems. This computation technique has ever been applied to control various factors on quality or operation of steel production. In this study, the neural network computation was applied to estimate viscosity and surface tension of mold fluxes.

As a result, the neural network computation reproduced accurately the experimental viscosity data in the multi-component systems for a wide range of SiO_2 content in mold fluxes. The accuracy in the estimation of the neural network computation was higher than that by the previous physical models such as Iida's model or Riboud's one. It also reproduced the literature data of the surface tension for binary and ternary molten silicate slag. Recently, the authors proposed a physical model for the estimation of the surface tension, modifying Butler's model considering ionic radii of components. Comparison of the evaluation by the neural network computation with that by the physical model was discussed in the present study.

INTRODUCTION

Physical properties of mold flux are very important factors for the control of various phenomena in a mold of continuous casting in steelmaking process. For example, since the viscosity is one of the main factors for the lubrication in the mold to keep productivity and surface quality of slabs, viscosity should be controlled to be optimum under each condition such as casting speed or steel grade. Viscosity, as well as surface tension, should be also controlled to prevent entrapment of mold flux into molten steel. Although the accurate evaluation of physical properties is required from the above view points, it is quite difficult to find appropriate data to apply directly to mold fluxes with complex compositions including SiO_2, CaO, Al_2O_3, MgO, Na_2O, Li_2O, CaF_2, etc. Thus, some estimation models based on physico-chemical theory have been proposed so far [1, 4], but there is no adequate model to estimate the physical properties for wide temperature and composition ranges in any kinds of multi-component mold fluxes.

Neural network computation is one of numerical estimation methods to cope with the above problems [5]. This computation has ever been applied to control various factors on quality or operation of steel production [6, 9].

In this study, the neural network computation was applied to estimate physical properties such as the viscosity and the surface tension of mold fluxes. Comparing the calculated results by the neural network computation with those evaluated by some physical models proposed so far, advantages and appropriate usage of the neural network computation are discussed [10, 11].

METHODOLOGY

Neural Network Computation

Neural network computation is an operation method modeled after neurons in human brain. Human brain is estimated to consist of about 10 billions of neuron [5]. As shown in Figure 1, a neuron consists of dendrite, soma, axon and synapse. Signal input from dendrites is recognized in the soma. When the intensity of the signal is higher than a certain critical value in soma, the output signal with stimulation is conveyed through the axon and the synapse to the next neuron. This transmission, called *ignition*, can be expressed in a sigmoid function expressed in Equation (1) in the neural network computation.

$$f(x) = \frac{1}{1+e^{-\eta x}} \tag{1}$$

Where x is a signal and $f(x)$ is an output, which gives unity for large x and zero for small x. η is a coefficient which specifies the shape of sigmoid curve shown in Figure 2. Applying this sigmoid function, computing sequence can be organized as neuron model.

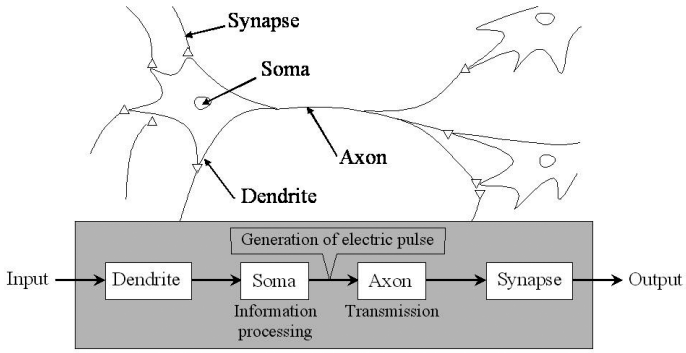


Figure 1: A concept of neuron

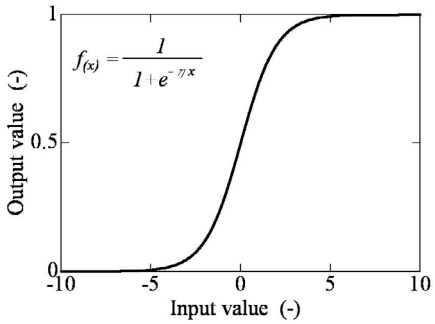


Figure 2: Sigmoid function

A concept of neuron model is shown in Figure 3. The neuron model consists of three layers: input layer, middle and output ones, respectively. The signal is translated in the input of x_1, x_2 and x_3 in the units of the input layer, and they are transmitted through the sigmoid function like *ignition* to middle layer for the first procedure. This calculation is expressed in Equation (2).

$$a_k = f(\sum x_i W_{ki} - W_{k0}) \tag{2}$$

Here, W_{ki} is connection weight, W_{k0} is a critical value and a_k is an output in the first procedure. a_k becomes input in the next procedure and gives the final output through the Equation (3).

$$y = f(\sum a_i V_i - V_0) \tag{3}$$

Here, V_{ki} is connection weight, V_{k0} is a critical value and y is the final output.

Connection weight is controlled so that the final output may converge to the teacher signal. A flowchart is shown in Figure 3. The final output is compared with the teacher signal and the difference between them is calculated as an error. The error is fed back to the connection weight by the Equations (4) and (5).

$$\Delta W_{ki} = -\varepsilon\alpha(y - t) \tag{4}$$

$$\Delta V_i = -\varepsilon\beta(y - t) \tag{5}$$

Then the calculation by Equations (2) to (5) is repeated in much iteration, as learning, till the error decreases so as to be less than a certain value given in advance. After all, the final output is given as an estimated result for each teacher signal.

When we try to evaluate physical properties such as surface tension, viscosity etc. by the neural network computation, the experimental conditions such as contents, temperature and pressure can be used as the input data. Experimental values of physical properties are used as the teacher signal, and the physical properties are calculated as the final output. Then, the calculated values are compared with the teacher signal. Using the finally decided values of the connection weight, it is possible to estimate physical properties for new arbitrary compositions of mold flux whose physical properties are unknown.

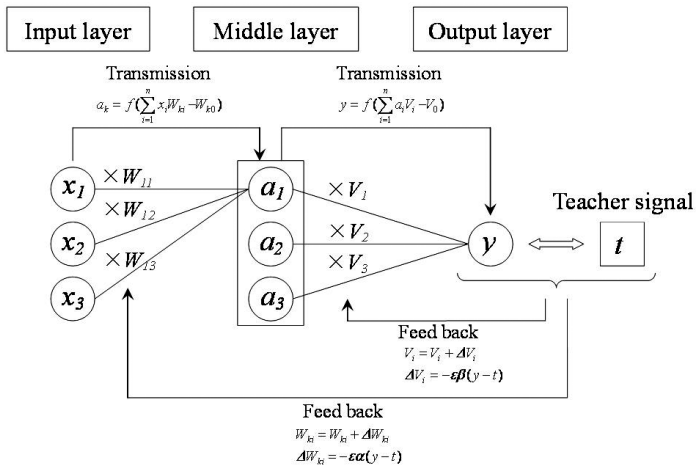


Figure 3: A flowchart of neural network computation

In the application of the neural network computation to the physical property estimation, there are some special characteristics, compared with physical models. There is no restriction on the number or sort of the components as input units. In addition, the components can be defined freely, without any physical meaning. For example, CaF_2 and NaF can be treated as they are, but even total F can also be accepted as an input data. Both of FeO and Fe_2O_3 can be defined as total Fe, in which we do not worry about their valencies.

Some different properties can be simultaneously estimated with high accuracy.

Calculating Conditions

Neural network computation was conducted with the software of *Neurosim/L* by Fujitsu Ltd. on the market in this study [12].

In the present calculation, the number of middle layer units, which is an arbitrary parameter in the software, was set at 5 or 6 and the calculation was repeated 200,000- 300,000 times for the convergence. The experimental values of viscosity or surface tension were used as the teacher signal.

Database

Surface tension of molten silicates or viscosity of mold fluxes was evaluated by the neural network computation in this study.

It is necessary to prepare databases on those physical properties with compositions

and temperatures for the evaluation by the neural network computation, and they were established in the present work as follows.

In the case of the surface tension, 467 of the experimental sample data were collected from the literature [13]. We selected silicate melts which were binary or ternary systems composed of Al_2O_3, CaO, FeO, MgO, MnO, Li_2O, K_2O, Na_2O or CaF_2. Their experimental data on the surface tension were quoted from the literatures [13].

On the database on viscosity, the viscosity of mold fluxes was measured with oscillating-plate viscometer [14] for 427 compositions in this study. These experimental values were used as the database on the viscosity of silicate melts. On the basis of 7-component silicate melt system of SiO_2-CaO-CaF_2-Al_2O_3-MgO-Na_2O-FeO, the other components such as B_2O_3, Li_2O, K_2O, MnO, P_2O_5 and TiO_2 were added to make additional 13-component systems.

RESULTS AND DISCUSSION

Estimation of the Surface Tension by Neural Network Computation

The calculated results on the surface tension of silicate melts by the neural network computation were compared with the experimental ones for all the samples in the database as shown in Figure 4. This Figure shows the results obtained from two steps of learning procedures. That is to say, after the first step learning of 300,000 iteration, the sample data, of which calculated final values had average errors more than 10%, were eliminated and then the second step learning was conducted for the remained samples. By means of this elimination, the evaluation became more precise and the average error defined in Equation (6) was evaluated to be about 2.5%.

$$\text{Average error} = \frac{1}{N}\sum_{1}^{N}\left|\frac{\sigma_{\text{cal},N} - \sigma_{\text{exp},N}}{\sigma_{\text{exp},N}}\right| \times 100 \qquad (6)$$

As an example, the calculated values of the surface tension of ternary CaO-SiO_2-FeO melt were compared with the experimental ones in Figure 5. The numerical figures in Figure 5 show the experimental values and those in round brackets indicate the eliminated data after the first step learning explained above. The estimated result of iso-surface tension curves agree well with the experimental values, but do not agree with the experimental values with round brackets so much.

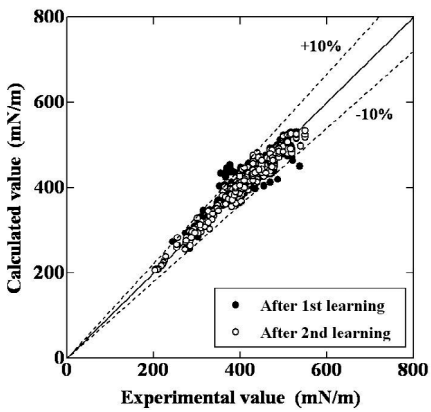


Figure 4: Comparison between calculated values of surface tension with experimental ones

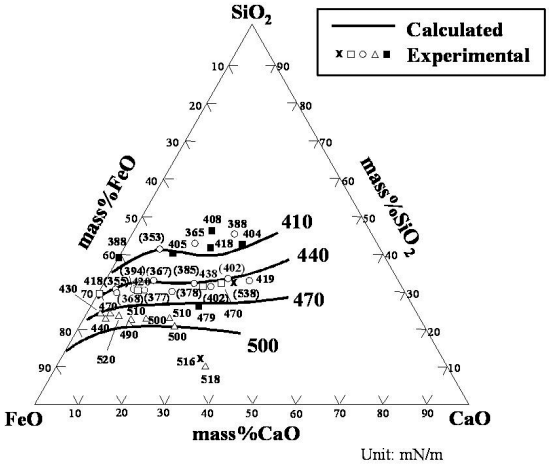


Figure 5: Surface tension of molten silicate in CaO-SiO_2-FeO ternary system

Comparison with Butler's Physical Model

Butler [15] derived an evaluation model of the surface tension for liquid solutions and this model was modified by Tanaka, one of the authors, to apply to molten ionic mixtures as shown in Equations (7) and (8) [16, 19].

$$\sigma = \sigma_{AX}^{Pure} + \frac{RT}{A_{AX}} \ln \frac{M_{AX}^{Surf}}{M_{AX}^{Bulk}} \qquad \sigma = \sigma_{BY}^{Pure} + \frac{RT}{A_{BY}} \ln \frac{M_{BY}^{Surf}}{M_{BY}^{Bulk}} \tag{7)(8}$$

Here, σ or σ_i^{Pure} are surface tension of binary molten ionic mixtures or pure component *i*, *R* is gas constant, *T* is temperature, *Ai* is molar surface area of pure component *i*, and is M_i^{phase}mole modified fraction with ionic radius in the *phase* of surface or bulk, as expressed in Equations (9) and (10) for each component of *AX* or *BY*, where *A* and *B* are cations and *X* and *Y* are anions. In these Equations, *Rj* is ionic radius of ion *j* and N_i^{phase} is mole fraction of component i in the *phase* of surface or bulk.

$$M_{AX}^{Phase} = \frac{\frac{R_A}{R_X} N_{AX}^{Phase}}{\frac{R_A}{R_X} N_{AX}^{Phase} + \frac{R_B}{R_Y} N_{BY}^{Phase}} \qquad M_{BY}^{Phase} = \frac{\frac{R_B}{R_Y} N_{BY}^{Phase}}{\frac{R_A}{R_X} N_{AX}^{Phase} + \frac{R_B}{R_Y} N_{BY}^{Phase}} \tag{9)(10}$$

This physical model has been used to evaluate the surface tension of molten slag in multi-component system. As an example, the surface tension of molten CaO-SiO_2-CaF_2 ternary system was evaluated by this model as shown in Figure 6(a). Dependence of the surface tension on CaO content was reproduced to agree with the experimental values.

On the other hand, the surface tension of the same system estimated by the neural network computation is shown in Figure 6(b). Compared with almost straight lines obtained by the above physical model in Figure 6(a), the iso-surface tension curves by the neural network computation fit the experimental values more faithfully.

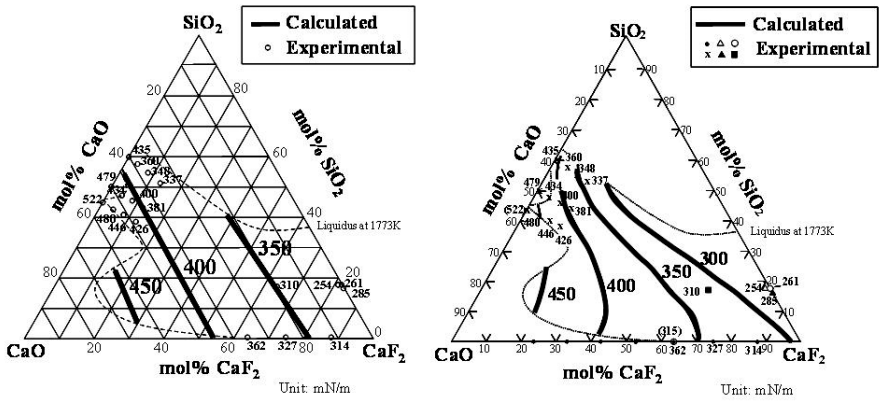


Figure 6: Calculated values of surface tension of molten silicate CaO-SiO_2-CaF_2 ternary system

Estimation of Viscosity by Neural Network Computation

The calculated results of the viscosity by the neural network computation are shown in Figure 7(a) for 7- component systems and 7(b) for 13-component systems. As shown in these figures, the accuracy of the estimation seems to be maintained even though the number of components in the systems changes from 7 to 13.

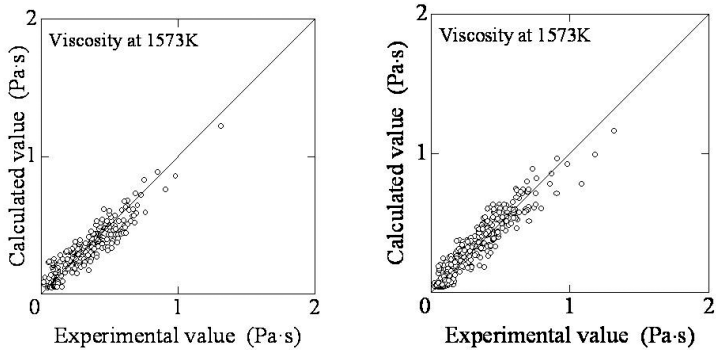


Figure 7: Calculated values of mold flux viscosity by neural network computation

Comparison with Physical Models

Several physical models of the viscosity of molten slag have been derived so far. For example, Riboud proposed the following physical model in Equation (11) [1].

$$\eta = AT \exp\left(\frac{B}{T}\right) \tag{11}$$

Here, T is temperature, A and B are parameters determined on account of experimental data and expressed in Equations (12) and (13).

$$A = \exp(-19.81 + 1.73X'_{CaO} + 5.82X_{CaF_2} + 7.02X'_{Na_2O} - 35.76X_{Al_2O_3}) \tag{12}$$

$$B = 31140 - 23896X'_{CaO} - 46356X_{CaF_2} - 39159X'_{Na_2O} + 38833X_{Al_2O_3} \quad (13)$$

Here, Xi is mole fraction of component i and X'i is calculated from Equations (14) and (15).

$$X'_{CaO} = X_{CaO} + X_{MgO} + X_{FeO_{1.5}} + X_{MnO} + X_{BO_{1.5}} \quad (14)$$

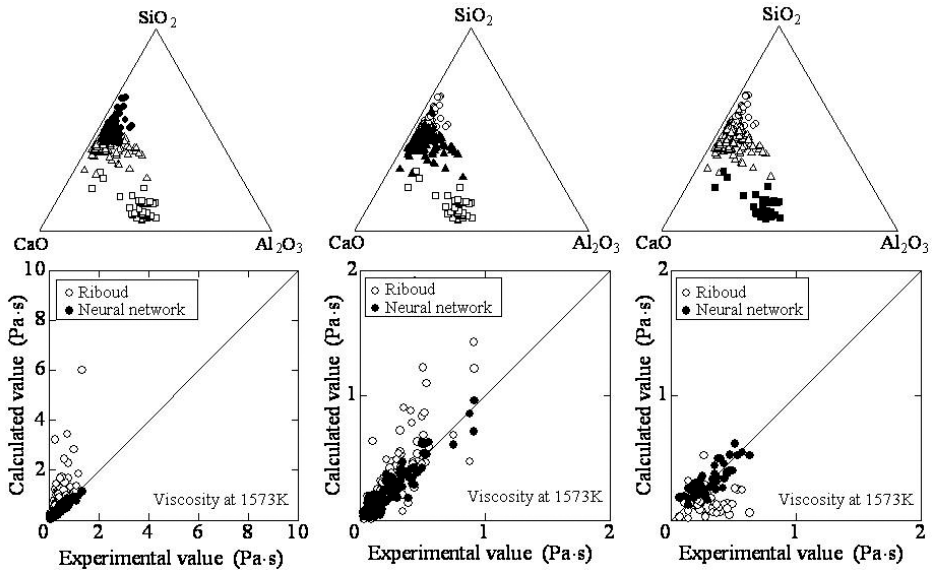
$$X'_{Na_2O} = X_{Na_2O} + X_{K_2O} \quad (15)$$

Figures 8 (a), (b) and (c) show the estimated results of the viscosity against the experimental ones, comparing between Riboud's model and the neural network computation. They were compared each other in the three grade of SiO_2 content in mold flux: (a) 40-60 mass%, (b) 20-40 mass% and (c) less than 20 mass%. In these Figures, the composition diagrams are also given to express the Al_2O_3 contents.

In comparatively high grade of SiO_2 content, in the Figure 8(a), the calculated values by Riboud's model show the tendency to be larger than the experimental ones, and the difference between them seems to become larger with SiO_2 content. On the other hand, the calculated values by the neural network computation agree well with the experimental ones.

In middle grade of SiO_2 content in Figure 8 (b), both of the calculated values agree with the experimental ones, although the smaller errors is available in the neural network computation compared with Riboud's model.

The calculated values by Riboud's model in low grade of SiO_2 content were smaller than the experimental values as shown in Figure 8(c). As shown in the composition diagram, Al_2O_3 content increases with the decrease of SiO_2 content. Al_2O_3, which is known to be amphoteric oxide, behaves as acid oxide when SiO_2 contents decreases, and this substitution of Al_2O_3 compensates the decrease of SiO_2 content to maintain the viscosity of mold flux. This behavior of Al_2O_3 is not reproduced adequately in Riboud's model. On the other hand, the calculated values by the neural network computation agree with the experimental ones.



(a) SiO_2 content: 40-60 mass % (b) SiO_2 content: 20-40 mass % (c) SiO_2 content: 0-20 mass %

Figure 8: Calculated values of viscosity of molten flux in 13 - component system

Appropriate Usage of Physical Models and the Neural Network Computation

As described above, the neural network computation reproduces the experimental values on the surface tension and the viscosity of molten slag more precisely than some previous physical models. The high precision is kept in the wide range of flux or slag compositions. The neural network computation can be a powerful technique in the estimation on the composition dependence of physical properties when highly reliable experimental data are available as teacher signals. Thus, in order to obtain higher precision, it is important to prepare reliable databases. On the other hand, even when we do not have any databases on physical properties, the physical models can be used to estimate the properties for a given new compositions or temperature. Consequently, we should use those two kinds of estimation techniques to suit our demands.

CONCLUSIONS

The neural network computation was applied to estimate the physical properties such as viscosity and surface tension of molten flux or slag, and it has been confirmed that the computation technique reproduced the experimental data precisely, compared with previous physical models.

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