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Evaluation of Viscosity of Mold Flux by Using Neural Network Computation

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A new estimation method of viscosity or solidification temperature of mold fluxes was proposed by applying the neural network computation. In this evaluation system, the viscosity and the solidification temperature of mold fluxes can be evaluated from the analytical compositions in multi-component systems of SiO_2–Al_2O_3–CaO–MgO–Na_2O–F–T.Fe–ZrO_2–TiO_2–BaO–MnO–B_2O_3–S–C without any conversion of S or F to sulphide or fluoride. It was found that the calculated results of the dependence of viscosity on temperature and composition agree with the experimental results more precisely than some conventional physical models for viscosity. Furthermore, viscosity of mold fluxes can be estimated precisely in the wide range of SiO_2 content.

KEY WORDS: viscosity; solidification temperature; slag; mold flux; neural network computation; regression; estimation.

1. Introduction

It is required to control viscosity of mold fluxes at molten state and there solidification temperature for the production of high quality steel by continuous casting processes. Therefore, we need precise information on the viscosity or the solidification temperature although mold fluxes have complex compositions in multi-component-oxide system including fluorine. If numerical estimation can be applied on the basis of enormous experimental data of the viscosity or the solidification of mold fluxes, it is useful to design a new composition of mold flux without measurements, and to carry out numerical simulations on some phenomena in continuous casting mold. Although there have been proposed various types of numerical models for the estimation of viscosity, precise estimation of the viscosity is quite difficult because of the following problems: Thus, SiO_2, which is one of the main components of mold fluxes, varies the viscosity in wide range and each component in mold flux also has some influences to the viscosity.[1] Furthermore, addition of amphoteric oxide such as Al_2O_3 lets the viscosity not only increase but also decrease,[1] and this influence of Al_2O_3 to the viscosity depends on the mold flux composition. That is why there have never been any numerical models of viscosity estimation that can successfully express the dependence of the viscosity on temperature and composition of the components in mold fluxes.

In this study, based on the experimental results of viscosity on several hundred kinds of mold flux, a new estimation method of the viscosity was constructed by the application of neural network computation, which can precisely regress the viscosity of mold fluxes as a function of inputs with multi-variables.

2. Neural Network Computation

Neural network computation is an operation method modeled after neurons which are as many as 10 to 14 billions in human brain.[2,3] As shown in **Fig. 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, an output signal with stimulation is conveyed through axon and synapse to the next neuron. The state that the intensity of signal exceeds the critical value is called "ignition". The signal cannot be conveyed until its intensity does not have ignition. These situation can be express in a sigmoid function shown in Eq. (1) in the neural network.[2,3]

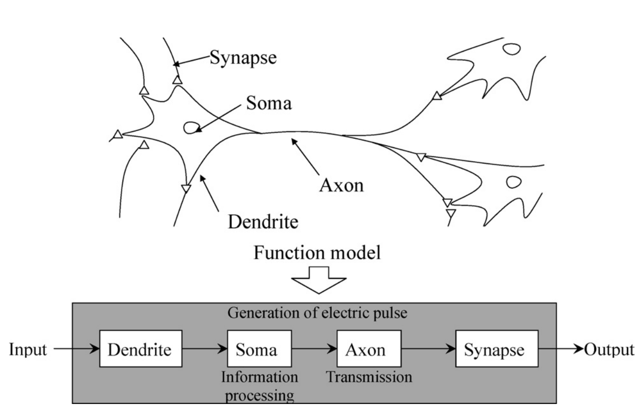


Fig. 1. A concept of neuron.

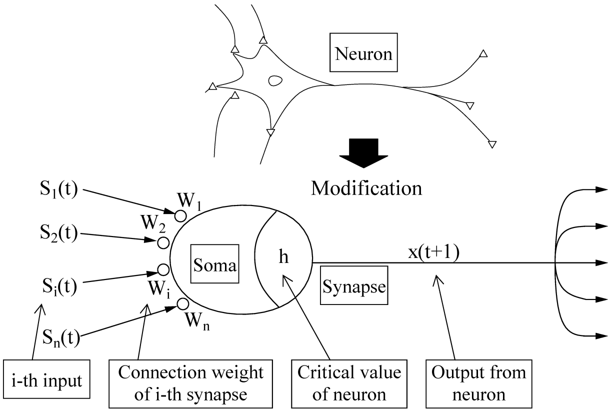


Fig. 2. Correspondence of neuron to neural network computer.

$$f(x)=\frac{1}{1+e^{-\eta \cdot x}} \quad \text{..............................(1)}$$

Where x is a signal and $f(x)$ is an output, which gives us unity for large x but zero for small x. η is a coefficient.

Figure 2 illustrates schematic views of the comparison of the neural network computation circuit with a neuron mentioned above. As shown in this figure, various input signals induce the ignition in the sigmoid function, and then the result that exceeds the critical value is conveyed as an output. In the layer-type neural network computation,[2,3] a middle layer with some units is generally equipped as shown in **Fig. 3**.

Input signals that exceed a critical value are conveyed through a sigmoid function to the middle layer. Then, new signals that exceed another critical value in the middle layer are conveyed to final outputs. In this process, cross terms among each original input data can be considered through the middle layer. An output value to the middle layer a_k is given in Eq. (2).

$$a_k = f\left(\sum x_i \cdot W_{ki} - W_{k0}\right) \quad \text{......................(2)}$$

Here, x_i is an original input value, W_{ki} is a connection weight, W_{k0} is a critical value, and $f(\sum x_i \cdot W_{ki} - W_{k0})$ is a sigmoid function in **Fig. 4**.
A final output value y is obtained by substitution of a_k in the following Eq. (3).

$$y = f\left(\sum a_k \cdot V_k - V_0\right) \quad \text{.........................(3)}$$

Here, a_k is an input value but it is also the output obtained in Eq. (2), V_k is a connection weight, V_0 is another critical value, and $f(\sum a_k \cdot V_k - V_0)$ is a sigmoid function mentioned above.

The final output value obtained by the above calculation is compared with a teacher signal. If the final output is different from the teacher value, this difference or an error is added to the previous connection weight, and then new calculation is conducted again as shown in **Fig. 5**. This modification method of the error is called Back Propagation Method.[2,3] The calculation is repeated until the difference between the output value and the teacher signal converges

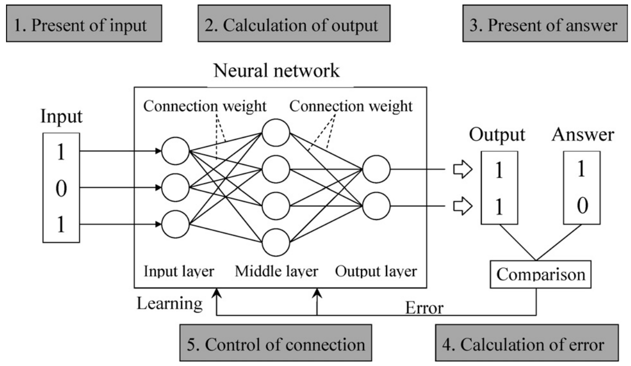


Fig. 3. Neural network model and organization of learning.

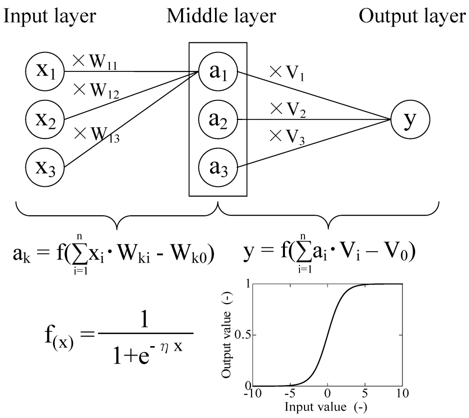


Fig. 4. Calculation of output values for middle and output layer.

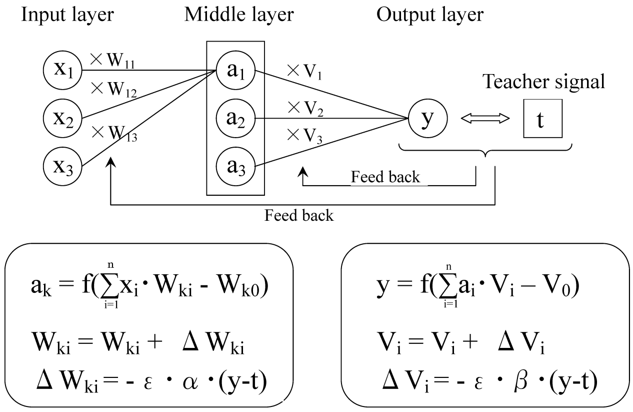


Fig. 5. Control of connection weight by feed back.

within a certain extent given in advance, and the final connection weights are determined. Using the function with the final connection weights, it is possible to estimate a new output value from arbitrary input data. This neural network computation has been being used for the evaluation of material properties in recent years.[4]

In the present study, regressions mentioned above were conducted for the experimental data of viscosity and solidification temperature of mold fluxes for continuous casting, which have several compositions in multi-component systems, with the software "Neurosim/L" produced by Fujitsu Ltd.[3] Then, the calculated results were compared with those of the conventional viscosity models as well as the experimental data.

3. Neural Network Computation for the Estimation of the Viscosity and the Solidification Temperature of Mold Fluxes

3.1. Application of Neural Network System to Regression of Mold Flux Viscosity by Using Round-Robin Project Data

At first, validity of the application of neural network system was examined by using the recommended data of mold flux viscosity obtained in the Round-Robin project.[5] This project offered reliable experimental viscosity data of molten oxides with their compositions and temperature. In addition, the project selected reliable prediction models of the viscosity, which reproduces the above experimental data precisely. It is reported by the Round-Robin project[5,6] that the following three models were proved to reproduce the experimental values of viscosity well, as a result of the examination of various viscosity estimation models proposed in the world:

(1) Seetharaman,[7] (2) Zhang,[8] (3) Iida.[9]

There remain some unsolved problems that the Iida's model needs experimental values to evaluate a parameter concerning to Al_2O_3, but it is more suitable model for the viscosity estimation of mold flux rather than two other models because it can be applied to multi-component system. In the present work, the highly reliable experimental data of the viscosity of mold fluxes recommended in the above Round-Robin project were used as input data to carry out the regressions by neural network computation. In addition, the calculated results by the neural network computation were compared with those by Iida's model against the recommended viscosity values for 142 compositions by the Round-Robin project.[4]

The data used here are viscosity values of mold fluxes with various compositions which consist of 14 components in SiO_2–Al_2O_3–CaO–CaF_2–Na_2O–MgO–Fe_2O_3–FeO–B_2O_3–Li_2O–K_2O–MnO–P_2O_5–TiO_2 systems. **Figures 6**(a) and 6(b) show the comparison of the calculated results by the neural network computation with the experimental values at 1 573 K (a) and 1 673 K (b). In these figures, we changed the number of units in the middle layer from 3 to 5. As shown in Fig. 6, the calculated results reproduce the experimental results precisely at different temperatures. The good results were obtained for all of three different unit numbers in the middle layer. Consequently, it is found that composition and temperature dependence of viscosity in multi-component systems can be evaluated simultaneously by the neural network computation.

Figures 7(a) and 7(b) show the comparison of the calculated results of the viscosity at 1 573 K (a) and 1 673 K (b) by the neural network computation for the number of 5

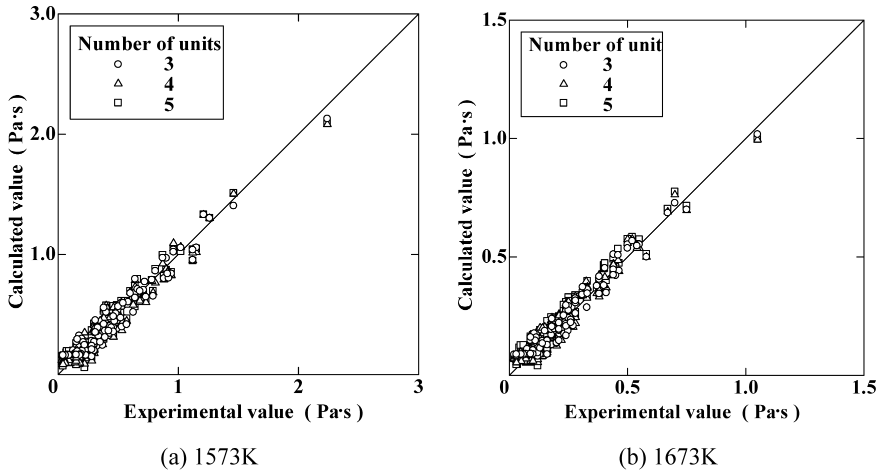


Fig. 6. Comparison between experimental value of mold flux viscosity and calculated one by neural network model.

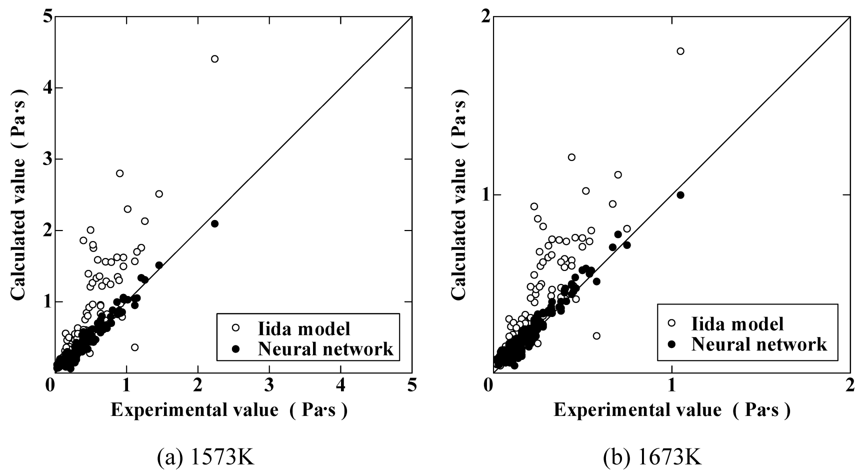
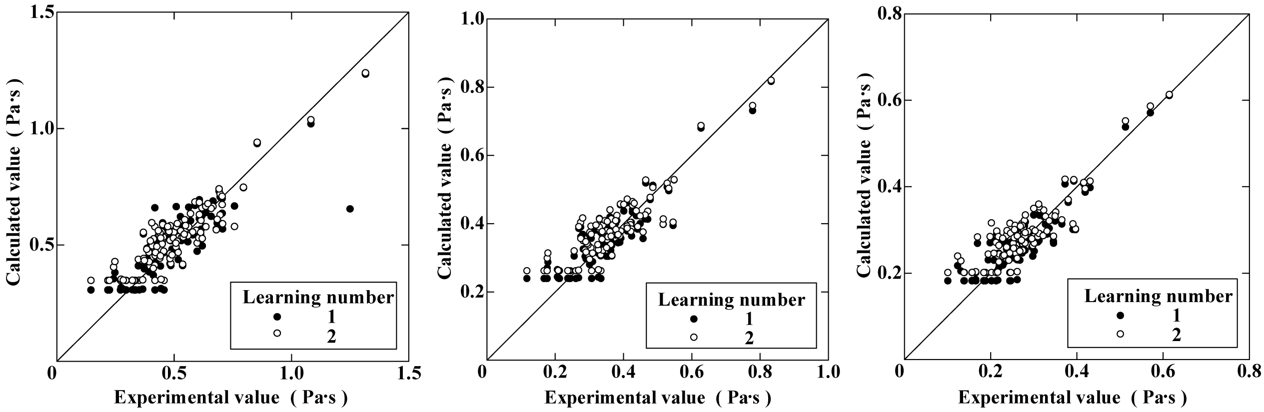
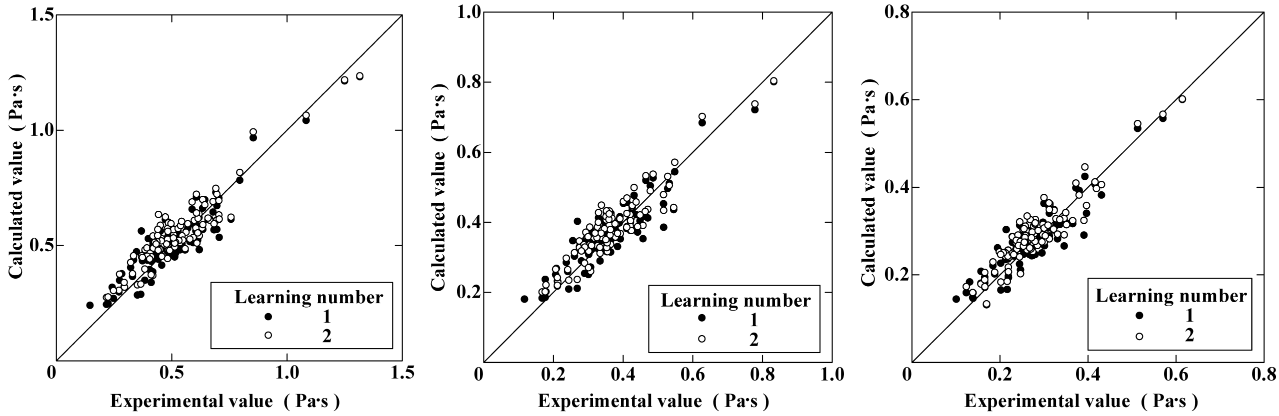


Fig. 7. Comparison between calculated value of mold flux viscosity by Iida model and that by neural network (number of unit is 5).



(a) 1573K (b) 1623K (c) 1673K

Fig. 8. Comparison between experimental value of mold flux viscosity and calculated value by neural network in the case that mold flux composition is 7-component-system and the number of unit is 3.



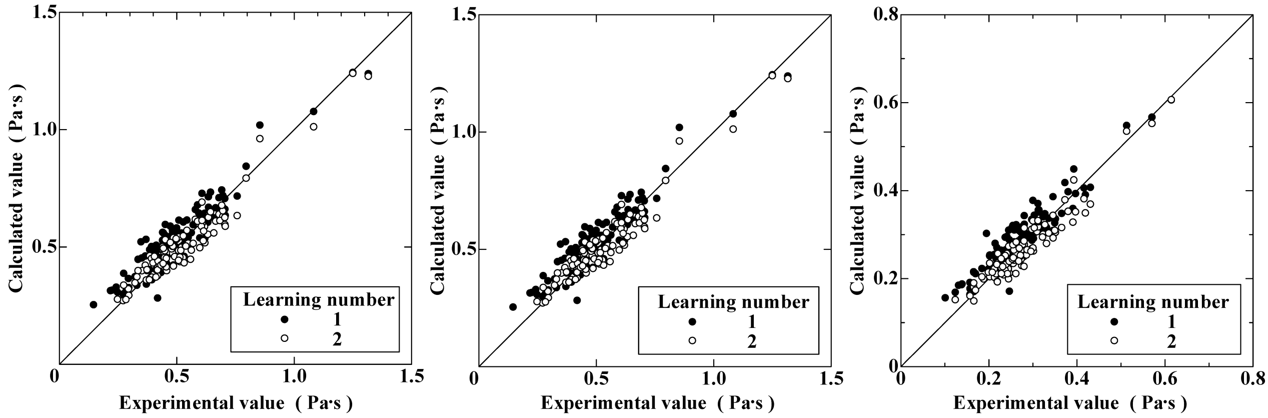
(a) 1573K (b) 1623K (c) 1673K

Fig. 9. Comparison between experimental value of mold flux viscosity and calculated value by neural network in the case that mold flux composition is 7-component-system and the number of unit is 4.

units in the middle layer with those by Iida's model. As shown in these figures, the reproduction by the neural network computation for the experimental values is extremely better than Iida's model, which was recognized to have good prediction in the Round-Robin project.

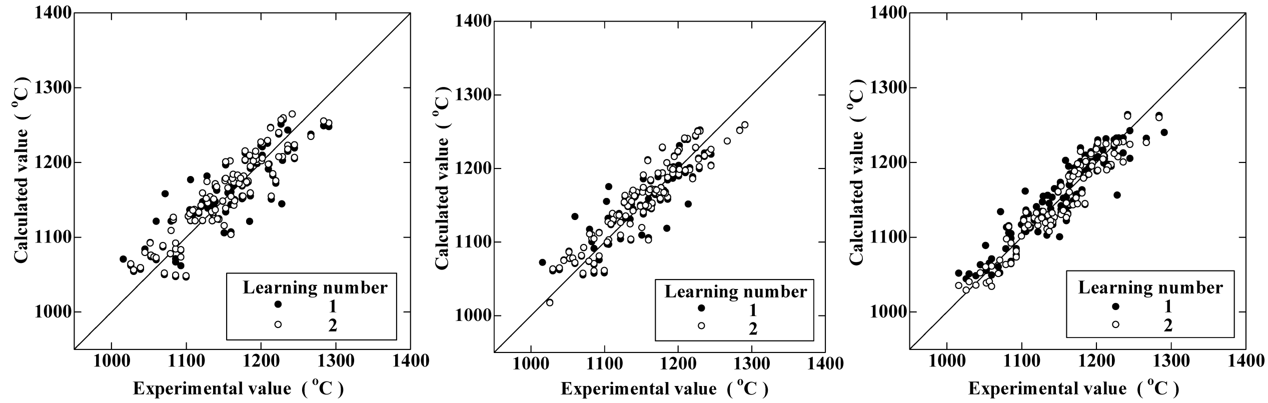
3.2. Simultaneous Calculation of Viscosity and Solidification Temperature of Mold Flux in 10-Component-systems

As mentioned in the preceding section, it is proved that viscosity can be estimated precisely by the application of the neural network computation. Then, regression calculation was conducted for our own experimental data of viscosity and solidification temperature of mold fluxes, which have been measured by an oscillating plate method[10] and accumulated in the authors' institute. At first, the calculation was conducted on the data of 109 compositions of SiO_2–Al_2O_3–CaO–MgO–Na_2O–F–T.Fe system, whose components were included in almost all the mold fluxes. **Figures 8**, **9** and **10** show the comparison between the experimental results and the calculated ones in the condition that the number of units in the middle layer was set to be 3, 4, and 5, respectively. In these figures, the plots indicated as learning number 1 were obtained from all of the original experimental values. In this calculation for these original experimental data, there are some scattered plots, which were supposed to contain some experimental errors such as precipitation of solid phases. Then, rejecting 5% of the data which have large error, the calculation was conducted again for the remaining data. The final results are expressed as learning number 2 in Figs. 8–10. The calculation was repeated 200 000 times at both cases of learning number 1 and 2, in which adequate convergence of the calculation was confirmed over 100 000 repeating times. As shown in Figs. 8–10, it is found that the experimental values can be reproduced precisely by the neural network computation, especially in the condition that the number of units in the middle layer was selected to be 5 in the learning number 2. **Figure 11** indicates the calculated results of solidification temperature obtained simultaneously with the above viscosity calculation. Solidification temperature was defined as the break point in the relation between $\log\eta$ and $1/T$, here η means viscosity of molten flux and T means temperature. As can be seen in this figure, precise regression was available in the condition that the number of units in the middle layer was selected to be 5 in the learning number 2.



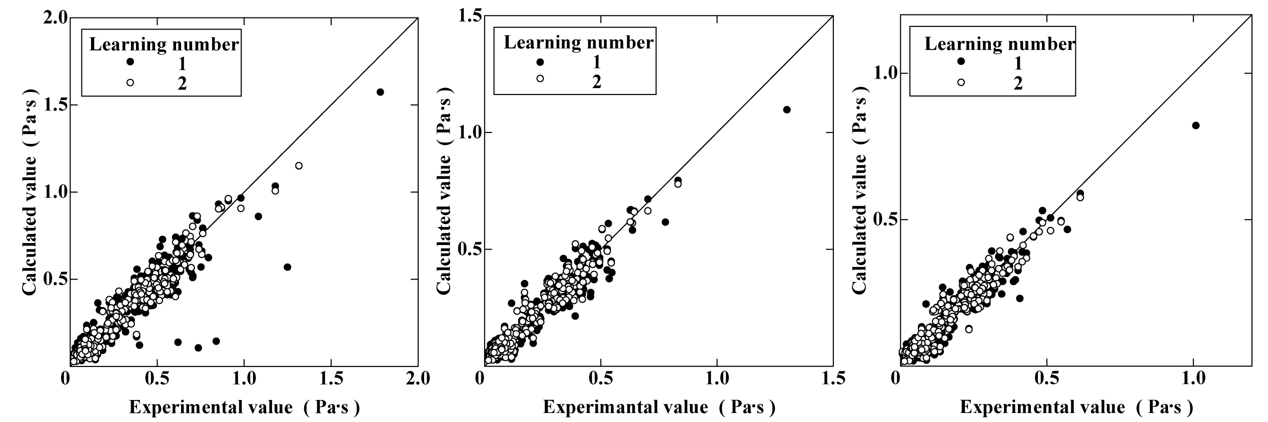
(a) 1573K (b) 1623K (c) 1673K

Fig. 10. Comparison between experimental value of mold flux viscosity and calculated value by neural network in the case that mold flux composition is 7-component-system and the number of unit is 5.



(a) Number of unit is 3 (b) Number of unit is 4 (c) Number of unit is 5

Fig. 11. Comparison between experimental value of solidification temperature of mold flux and calculated value by neural network in the case that mold flux composition is 7-component-system.



(a) 1573K (b) 1623K (c) 1673K

Fig. 12. Comparison between experimental value of mold flux viscosity and calculated value by neural network in the case that mold flux composition is 15-component-system and the number of unit is 5.

3.3. Simultaneous Calculation of Viscosity and Solidification Temperature of Industrial Mold Fluxes in 15-Component-systems

In this section, the regression calculation by the neural network computation was conducted for 344 data in 15-component-systems of SiO_2–Al_2O_3–CaO–MgO–Na_2O–F–T.Fe–ZrO_2–TiO_2–BaO–MnO–B_2O_3–S–C, which cover various industrial mold fluxes. The calculated results were shown in **Fig. 12**. It was clarified from this figure that even in the condition for enormous data of multi-component-system, good regression could be conducted to give precise viscosity estimation. In addition, it should be remarkable that the analytical values of F, T.Fe or S can be used directly as input data without any conversion to the composition of their compound as CaF_2, FeO or Fe_2O_3, FeS *etc*. **Figure 13** shows the comparison of the calculated results from the neural network computation with those by Iida's model for

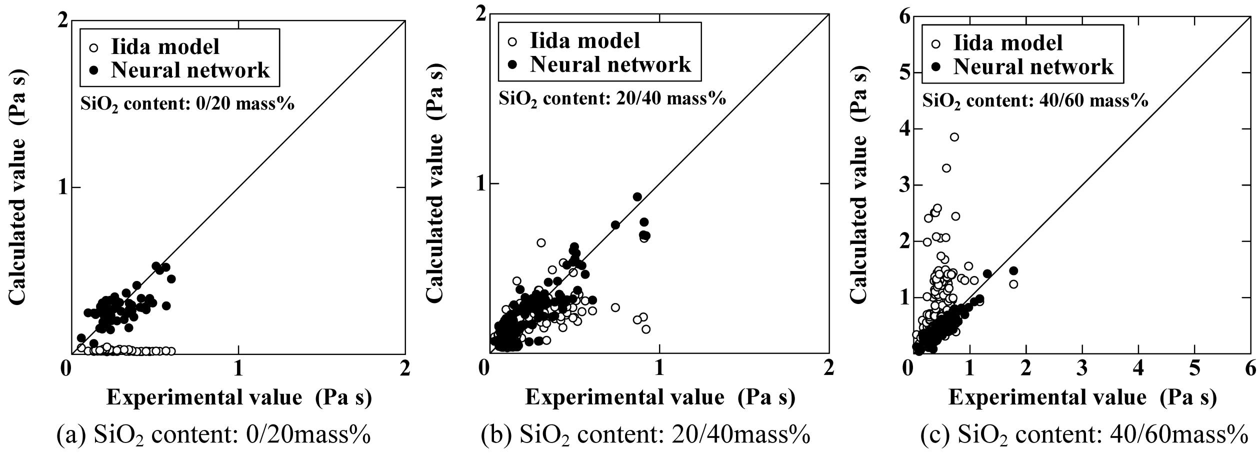


Fig. 13. Comparison between experimental value of mold flux viscosity and calculated value by neural network in the case that mold flux composition is 15-component-system and the number of unit is 5.

three different SiO_2 content ranges in mold fluxes. As shown in Fig. 13(a) for SiO_2 content less than 20 mass%, the calculated values by Iida's model tend to be lower than the experimental values. In the range that SiO_2 content is more than 40 mass%, the calculated values by Iida's model show higher than the experimental values as shown in Fig. 13(c). On the other hand, the neural network computation agrees well with the experimental values in wide SiO_2 range.

4. Conclusions

In the present work, we applied the neural network computation to the prediction of the viscosity and the solidification temperature of mold fluxes in multi-component systems. It was found that mold flux viscosity can be estimated quite precisely by the neural network computation, in comparison with the estimation by conventional physical models. On the basis of the present results, the estimation system, which reproduces the experimental data of viscosity and solidification temperature of mold fluxes precisely, can be constructed by the neural network computation.

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