# VISCOSITY PREDICTION OF C-A-S AND C-A-S-M-SLAG SYSTEMS BY MEANS OF AN ARTIFICIAL NEURAL NETWORK*

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**Abstract**
Slags are of fundamental importance in the steel production, influencing deeply its quality; among the several properties of steelmaking slags, viscosity stands out as one of the most important. Viscosity is a function of slag composition andtemperature and is determined experimentally or using mathematical models.In this work a study is made todetermineviscosity by means of an Artificial Neural Network using Wekasoftware developed at the University of Waikato.Weka offers several algorithms for machine learning, including those for neural network training. Here, the Multilayer Perceptron model (MLP) was used andtraining was carried out by means of the error back-propagation algorithm. For this introductory analysis, the composition of the chosen slags falls within the most frequently used quaternary oxide system CaO-MgO-$SiO_2$-$Al_2O_3$ (also known as C-S-A-M) and the ternary C-S-A, while the temperature is kept constant at 1600 °C.Because of the facilities offered, the primary viscosity input data for selected slags was provided by means of FactSage – a software specialized in the field of metallurgical thermodynamics (nevertheless, literature or experimental data can be used as well). A refined predictive system for viscosity could be established by ANN with correlation coefficients between predicted and observed values ($R^2$) greater than 0.99 for both systems. The model can be of benefit to the steel industry and may contribute to the production of quality steels.
**Keywords:**Artificial neural network; Viscosity; Slags; C-S-A-M system.

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## 1. INTRODUCTION

The area of Science known as transport phenomena deals with the transfer of *momentum*, *heat* and *mass*. The *flux* of any of these properties is proportional to a distinct driving force gradient – in the first case, for Newtonian fluids, the proportionality constant is called *viscosity*. When studying slags, viscosity, together with thermal diffusivity, density, and interfacial tension, comprise the four most important thermo-physical properties. In order to have the necessary metallurgical operations running smoothly, molten slags and fluxes of moderate viscosities are needed. The viscosity of liquid oxides ismainly a function of their chemical composition and temperature; in steel mills, slags are used at elevated temperatures, yet the range – between 1250 and 1700 °C –suggests the existence of a wide amplitude of viscosities. Even for fixed temperature and composition, viscosity may still be affected by the presence of solid particles randomly dispersed in the liquid (this case will not be considered in this work). As for the composition, one can say that among the most common slag systems to be found in steelmaking thereare the quaternary oxide system $CaO$-$SiO_2$-$Al_2O_3$-$MgO$ (also known as C-S-A-M), together with its subsystem C-S-A.

Viscosity is measured experimentally or may be determined theoretically. Traditionally, viscosity has been measured using a wide range of experimental techniques developed over the past years,depending on the type and temperature of the liquid phase. Due to the high temperatures used in steel production processes, some methods have preference. For molten slags and fluxes, the most common are: the capillary method, the dropping body method, and the rotating cylinder method. They are based, respectively, on the flow time a portion of the fluid needs to pass through a thin channel; on the time required for a falling sphere immersed in the liquid to reach the melting pot bottom, and finally in the torque required to rotate a cylindrical component immersed in the fluid. A detailed description of these and some other methods used in the determination of slag viscosities can be found in Slag Atlas [1].

After the experimental measurements, a variety of mathematical models are applied to the data in order to create a scheme capable of predicting viscosity from composition and temperature. An excellent description of the various mathematical models used to describe the viscosity of metallurgical oxide melts is presented by Kekkonen *et al.* in a booklet under the general title of *Viscosity Models for Molten Slags* [2].

While mathematical models are essentially empirical in nature, a new method has emerged, based on a very different approach, *i.e.*, on the internal *structure* of slags. It is a well-known fact that the addition of basic oxides reduces the viscosity of molten silicates due to the breaking of the silicate network; viscosity thus reflects the internal structure of the molten oxide. This feature was incorporated into the commercially available software FactSage (developed by CRCT and GTT), whichdelivers viscosity directly as an output [3]. Yet another thermodynamically-related method is cited in the literature(based on the Gibbs activation energy for viscosity), and is incorporated in the software Thermoslag (developed at the Royal Institute of Technology, KTH) [4].

Accurate viscosity estimates, however, are still difficult to obtain, despite the advancement of the mathematical models, or the use of thermodynamic computational tools. Thus, some authors have proposed the use of artificial neural networks (ANNs) to accomplish this[5, 6, 7] and other tasks in the field of metallurgy

[8, 9, 10]. Neural networks applied in the prediction of viscosity do not need a description of the strong influence of silica, they do also circumvent the contradictory action of amphoteric oxides such as alumina, and avoid the determination of slag structures (required on thermodynamic-basedmodels). Because of this, ANNs do not present the limitations and assumptions of these models;consequently, they may provide results that can be regarded as 'neutral' or devoid of bias.
In the present work, an ANN approach has been used to predict viscosities of slag compositions in $CaO\text{-}SiO_2\text{-}Al_2O_3$and $CaO\text{-}SiO_2\text{-}Al_2O_3\text{-}MgO$ systems with an objective to establish an exploratory, though reliable, predictive system.

## 2.METHODOLOGY

Weka [11] is an artificial intelligence program developed at the University of Waikato, New Zealand; because of its performance and availability, it has been chosen for this work. Weka is a collection of *machine learning* algorithms for data mining tasks; the algorithms can be either directly applied to a dataset or called with a Java code; it contains tools for data pre-processing, classification, regression, clustering, association rules, and visualization, andit is also well-suited for developing new machine learning schemes.
Before applying the software it is necessary to fulfill (basically)three steps: i) data collection; ii) data normalization; and, iii) ANN configuration.

i) Data collection
Two datasets were used in this research,both of them constructed by means of the software package FactSage (and its database for 'melts'; the slag *structure* is calculated from the thermodynamic description of the melt using the Modified Quasichemical Model). The first is designed to describeslagsfrom the ternary system C-S-A and the secondslags from the quaternary system C-A-S-M.
This choice of input data preparation offers the advantage of rapidly constructing viscosity datasets that are 'evenly spaced'in composition– this would be much more difficult to dowith literature sources such as Slag Atlas [1]. In this case, composition values would be more erratic (*i.e.* non-regularly spaced), since isoviscositylines in diagrams rarely coincide with composition grid nodes. Conversely, the reading of the composition would entail some inaccuracy, because diagrams are usually 'drawings', tend to be small in size, and show onlymain grid lines (if any).
However,eventual deviations between experimental and 'software viscosities'will not impair the applied method – although they are undesirable.
Input data for the determination of slag viscosity by neural networks refer to slag compositions in terms of the four simple oxides: *silica*, *alumina*, *calcia* and *magnesia*plus viscosity (given in the International System units: Pascal second, or Pa·s). The chosen systemsparticularly reflect the melt shop practice, reduced in this work to the three (C-S-A) or four (C-S-A-M) oxides that most suitablyrepresent them. All viscosity data supplied as input refer to the temperature of 1600 °C; it is important to mention that data is restricted to those compositions that give rise to a single-phase *liquid* slags – at that temperature. Viscosities of slags containing *solid* phases in suspension should be corrected by means of equations such as the Einstein-Roscoe model, which takes into account the volume fraction of the solids. To avoid unnecessary route deviations, these bordercompositions were meticulously discarded andset as boundariesfor the actually usable composition field.

b) Data normalization

The data provided have values outside the usable range -1 and 1, so there is a need for normalization. One can use Weka's available normalization algorithm, or do this through the Multilayer Perceptron algorithm itself. In order to better visualize the results output, the normalization algorithm option was chosen, since it normalizes the data only for internal use, that is, the data is initially normalized, then used by the neural network, and at the end is reconverted, so that both reading and analysis are facilitated.

c) ANN configuration

Wekahas to be configured to perform the training of the multilayer perceptron (MLP) network. In order to configure any neural network, a series of non-trivial decisions must be made, so that the ANN presents satisfactory results. Among those of main importance are: network topology, learning algorithm (in this case the choice fell on the *back-propagation algorithm*), and activation function. Configuration includes the definition of the following parameters: number of hidden layers; learning rate; momentum; training time; and training set.

There are several methodologies to perform these tasks; often the choices are made empirically, so that the configuration of the neural network comes to be considered by many as an 'art'. Experience is required from the designers in order to getadequate results from the artificial neural network.

The MLP network can be trained by the back-propagation algorithm to perform any mapping between the input and the output values. The back-propagation algorithm searches for weight values that minimize the total error of the network over the set of training examples (training set). The choice of the number of layers in the Weka back-propagation algorithm can be done in two ways: manual or automatic; for simplicity, the automatic mode was selected. Three main parameters were adjusted during configuration: learning rate, momentum and training time. For configuration purposes, Weka standards were initially used, with a learning rate of 0.3, a momentum of 0.2, and a training time of 500. Adjustments consisted of fine tuning, performed empirically, accordingly to the output value $R^2$. The amount of data used for learning was: 55 and 76 input vectors (composition and viscosity) for C-S-A and C-S-A-M systems, respectively. Since this amount of available data is relatively small, a 10-fold cross validation (CV) was used.This means that Weka picks up 90% of the sample randomly and uses it to train, while 10% is used for validation. This procedure is performed a total of 10 times, creating a set of training and validation data.The advantage of this method is that all observations are used for both training and validation, and each observation is used for validation exactly once.No other manual adjustments have been made.

## 3. RESULTS AND DISCUSSION

Onceall stagesare accomplished, the artificial neural network is able to be applied andto predict the viscosity values, at 1600 °C, as a function of the input data (in this case, the slag composition).The ANN evaluation can bedone using appropriate error measures to interpret the results.Wekasoftware provides a general adequacy evaluation table of the ANN for the job (correlation coefficients plus errors). A graphical analysis of the results mayalso be easily made by observing the diagrams of the predicted viscosities by the artificial neural network plotted as a function of the input viscosity values (provided by FactSage software),regardless of composition.

These diagrams,together with the several numerical outputs(squared-R plus absolute and relative errors)will be presented and analyzed in the sequence for each of the two focused slag systems.

### 3.1 C-S-A system

The predicted viscosities plotted as a function of the input viscosity data,in the C-S-A systemcan be seen in Figure 1. Most of the input points lie in the lowerrange, up to approximately 3 Pa·s – which are reasonable adequate values, expected for metallurgical slags; from the figure, the relationship between predicted and input values is apparentlysuperior.
The correlation coefficient, $R^2$, obtained from the comparison between predicted and input values was, for this system, 0.9998,which means that the neural network has learned from input data and is able to predict the viscosity of anyslag compositionin the allowed range inthe C-S-A system, at a temperature of 1600 °C,with a high degree of accuracy. The relatively low errors confirm the good quality of this prediction. The general adequacy of the ANN model is presented in Table 1.

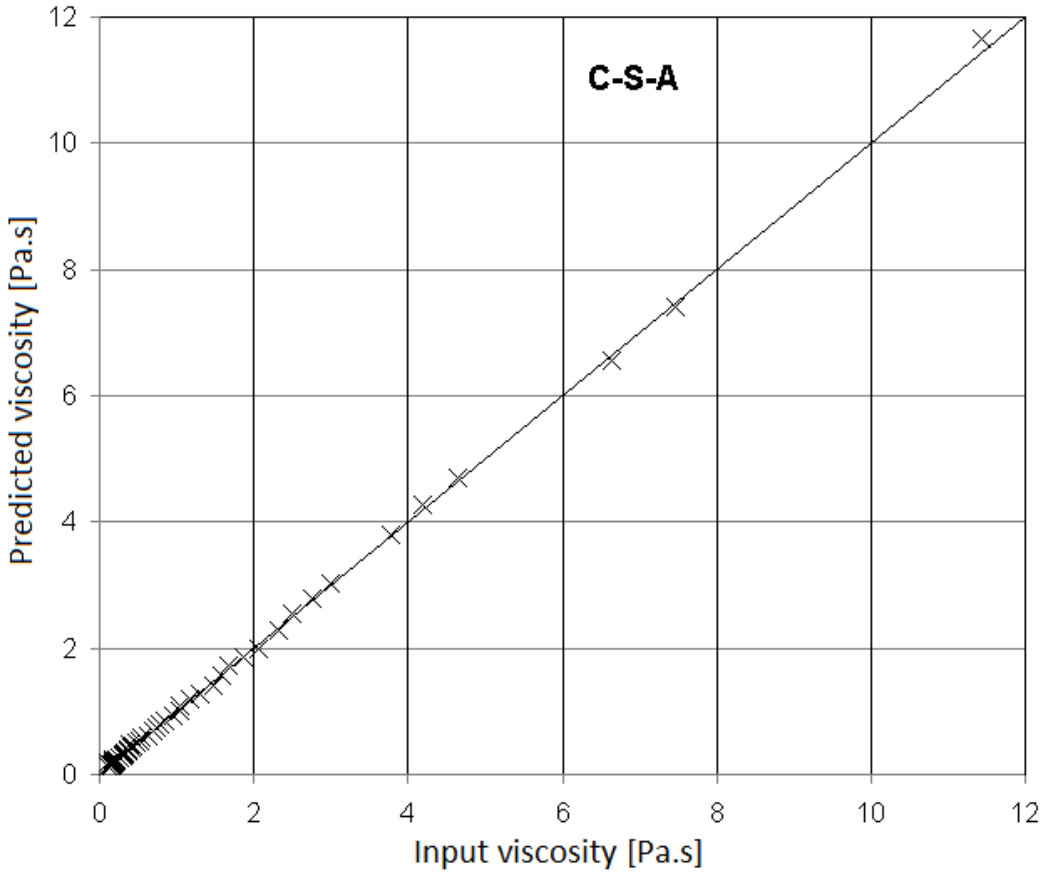


**Figure 1.** Predicted viscosity values as a function of the input values, C-S-A system

**Table 1.** Correlation coeficient $R^2$ and errors, C-S-A system

| Parameter | Value |
|---|---|
| Correlation coeficient | 0.9998 |
| Mean absolute error | 0.0295 |
| Root mean squared error | 0.0452 |
| Relative absolute error | 2.1292 [%] |
| Root relative squared error | 2.1096 [%] |
| Total number of instances | 55 |

### 3.2 C-S-A-M system

Also the predicted viscositiesin the C-S-A-M system, plotted as a function of the input viscosity data, can be seen in Figure 2. Here, the relationship between the predicted and input values is again noticeably good, especially for values smaller than 1.2 [Pa·s].
The correlation coefficient $R^2$ obtained from the comparison between predicted and inputvalues was, for this system, 0.9972. As for the previous system, again, theANN predictedsuccessfullythe viscosity valuesfor any (allowed) composition in the C-S-A-M system at a temperature of 1600 °C. The errors are also relatively low, which confirms the good quality of the prediction. The general adequacy of the ANN model to predict viscosities in the C-A-S-M slag system is presented in Table 2.

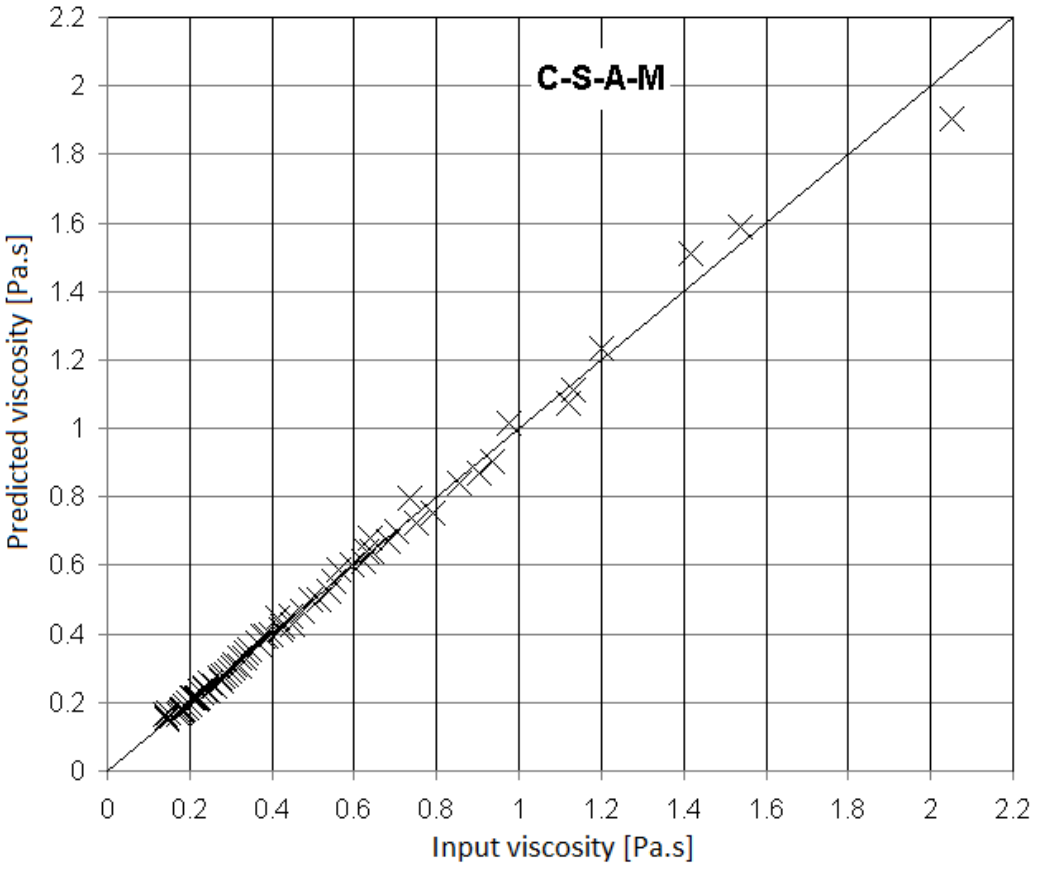


**Figure 2.** Predicted viscosity values as a function of the input values, C-S-A-M system

**Table 2.** Correlation coeficient $R^2$ and errors, C-S-A-M system

| Parameter | Value |
|---|---|
| Correlation coeficient | 0.9972 |
| Mean absolute error | 0.0154 |
| Root mean squared error | 0.0268 |
| Relative absolute error | 5.8881 [%] |
| Root relative squared error | 7.4308 [%] |
| Total number of instances | 76 |

## 3. CONCLUSIONS

From the results it can be concluded that, for metallurgical slagsbelongingeither to the C-S-A or to the C-S-A-M systems, in the fully *liquid* condition, and at the single temperature of 1600 °C,viscositydetermination usingan artificial neural network proved to be a powerful tool, despite of its low use, showing a strong linear relationship between predicted and observed values.

Results obtained with input data from the C-S-A ternary system are slightly better ($R^2$ = 0.9998) than those from the quaternary system C-S-A-M ($R^2$ = 0.9972) – possibly due to the smaller number of composition variables and thesmaller amplitude of the related data. Even so, the quaternary system had its viscosities nicely predicted – especially in the lower range of values – within the errors, considered to be low.

Summarizing,a refined predictive system for viscosity could be established by an ANN model; a largerversionwould be of benefit to the steel industry and thus may contribute for the production of qualitysteels.

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