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LINEAR MODELING AND FEATURE SELECTION OF BREAK TEMPERATURE IN MULTICOMPONENT SLAGS

Patrick Queiroz dos Anjos[1*], Lucas de Almeida Quaresma[1], Marcelo Lucas Pereira Machado[1]

1 — Federal Institute of Espírito Santo (IFES) – Vitória, ES.
patrick.dosanjos@outlook.com

ABSTRACT

Break temperature (T_{br}) is one of the most important parameters in slag, considered one of its critical factors, indicating the beginning of the loss of its fluidity. A literature database was built to establish a relationship between the chemical composition of the slag and the prediction of its T_{br}, both experimentally measured, through mathematical modeling by linear regression with L1 regularization (or Lasso). The resulting model, called L1 Model, resulted in lower deviation maximum error, mean and variance in relation to the T_{br} values of the database. Sensitivity analysis was performed to present the correlations between chemical composition and T_{br}.

Keywords: *Break Temperature, Chemical Composition, Linear Regression, Sensitivity Analysis*

INTRODUCTION

Slags applied on continuous casting processes have some essential characteristics, such as viscosity at a temperature of 1300°C, percentage of solid crystallized layer inherent to the mold and break temperature (T_{br}), the latter considered as the third critical parameter for these slags[(1)].
The T_{br} can be defined as the point where there is a significant increase in viscosity in which the slag shows a non-Newtonian behavior in a cooling, measured experimentally in viscosity measurements[(2)].
Considered as an indicator reference where the slag begins to lose fluidity[(3)], the T_{br} can be mathematically modeled by linear regression methods[(4)].
The purpose of this work is to model mathematically the T_{br} through the linear regression method with feature selection through a literature database.

MATERIALS AND METHODS

A literature database[(5-11)] was used, consisting of 54 different chemical composition data with their T_{br} experimentally measured. Thus, the predicted variable T_{br} (K) was mathematically modeled by linear regression with regularization L1[(12)] method (or *Lasso*) (Equation (A)) with feature selection using the chemical composition (%mass) composed by chemical system CaO-SiO_2-Al_2O_3-MgO-Na_2O-Li_2O-B_2O_3-MnO-TiO_2-FeO-K_2O-Cr_2O_3-CaF2 considered the predictor variables.

The values resulting from the applied mathematical modeling were compared with equations Steady State Condition Model and Dynamic Condition Model[4] through statistical evaluations of maximum error and the first and second central moments[13] (mean and variance, respectively) of the deviations, considered as the differences between the predicted values, resulting from linear regression and literature equations, and the database values. Subsequently, a sensitivity analysis was performed on the results of the mathematical modeling as a function of the relationship between chemical composition and T_{br}.

$$\text{minimize } ||Ax-y||^2_2 + \Sigma\, a||x||_1 \quad (A)$$

(*A* is the vector of the constants related to each chemical species of the chemical system of the database (dimensionless), *x* the vector of the chemical species of the chemical composition (%mass), *y* the values of T_{br} (K) and *a* the regularization parameter L1 (dimensionless))

RESULTS AND DISCUSSION

The parameter *a* that presented the smallest deviations obtained the value of 2. The linear model, named *L1 Model*, can be seen in Equation (B).

$$T_{br}\,(K) = 413.9 + 12.08\%CaO + 0.05\%SiO_2 - 16.80\%MgO + 13.11\%Na_2O + 1.2\%Li_2O - 15.22\%B_2O_3 - 11.90\%TiO_2 + 27.87\%FeO - 2.48\%CaF_2 \quad (B)$$

The graph relating the values predicted by the L1 Model, Steady State Condition Model and Dynamic Condition Model[4] can be seen in Figure 1.

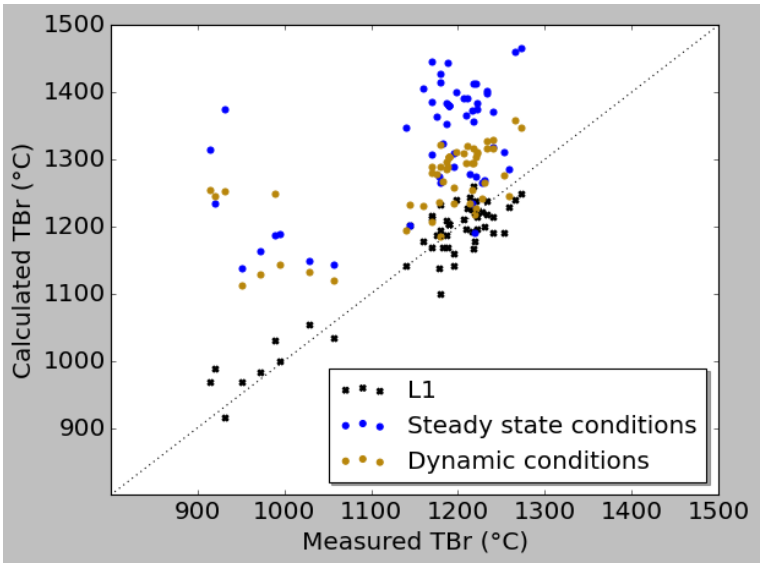

Figure 1: Predicted values of L1 Model, Steady State Condition Model and Dynamic Condition Model[4].

The deviation maximum error, mean and variance results can be seen in Table 1. The L1 Model resulted in a lower maximum deviation, mean and variance, in relation to the Steady State Condition Model and Dynamic Condition Model[4] equations.
CaO, SiO_2, Na_2O, Li_2O and FeO are chemical species that increase T_{br} and MgO, B_2O_3, TiO_2 and CaF_2 are chemical species that decrease T_{br} in L1 Model. The presentation of null values for the constants related to the chemical species Al_2O_3, MnO, K_2O and Cr_2O_3 correspond to the feature selection and present null sensitivity in relation to T_{br}. That is, any variation between

the chemical species Al_2O_3, MnO, K_2O and Cr_2O_3 does not correspond to a variation in T_{br} in linear regression with L1 regularization method.

Table 1: Statistical Evaluation of deviations in L1 Model, Steady State Condition Model and Dynamic Condition Model[4].

Statistical Evaluation	Deviation Max. Error (°C)	Deviation Mean (°C)	Deviation Variance (°C²)
L1 Model	79.89	26.44	360.01
Steady State Condition Model	442.73	163.47	7138.04
Dynamic Condition Model	340.61	98.26	5143.70

CONCLUSIONS

• A literature database was used to perform linear regression by L1 regularization to relate the chemical composition variables (%mass) composed by the chemical system CaO-SiO_2-Al_2O_3-MgO-Na_2O-Li_2O-B_2O_3-MnO-TiO_2-FeO-K_2O-Cr_2O_3-CaF_2 with break temperature (T_{br}) (K), obtaining the mathematical model L1 Model.
• The L1 Model obtained the lowest deviation maximum error, mean and variance in relation to the other 2 equations in the literature.
• CaO, SiO_2, Na_2O, Li_2O and FeO increase T_{br}, MgO, B_2O_3, TiO_2 and CaF_2 decrease T_{br} and Al_2O_3, MnO, K_2O and Cr_2O_3 present null sensitivity in relation to T_{br} in L1 Model.

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