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Modeling and Prediction of the Melting Temperature of Soda-Lime Glasses Based on Their Chemical Composition Using Artificial Neural Networks

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Abstract

The melting temperature of soda-lime glasses is a key processing parameter that governs energy consumption, melt viscosity, and manufacturing cost. Owing to the highly nonlinear relationship between glass composition and melting behavior, accurate prediction of melting temperature remains challenging. In this study, an artificial neural network (ANN) was developed to predict the melting temperature of glasses in the SiO_2-Na_2O-CaO ternary system directly from their chemical composition. A database containing 45 unique compositions collected from the literature and experimental studies was used for model development. The ANN employed the molar fractions of SiO_2, Na_2O, and CaO as input variables and the melting temperature as the output. The proposed 3-10-10-1 feed-forward architecture achieved a mean absolute error (MAE) of 2.74˚C and a root mean square error (RMSE) of 4.66˚C on the training dataset. External validation yielded an MAE of 18.29˚C and an RMSE of 20.68˚C, while an additional validation using independent experimental data reported by Santoso *et al.* confirmed the predictive capability of the model, with an MAE of 14.35˚C and an RMSE of 19.12˚C. These results demonstrate that the proposed ANN accurately captures the relationship between chemical composition and melting temperature and constitutes a reliable and efficient tool for the preliminary design and optimization of soda-lime glass compositions, thereby reducing the need for extensive experimental investigations.

Keywords

Soda-Lime Glass, Melting Temperature, Artificial Neural Network, Machine

Learning, SiO_2-Na_2O-CaO Ternary System

1. Introduction

Soda-lime glasses represent the most widely produced family of glasses worldwide and account for approximately 90% of industrial glass production [1]. Owing to their transparency, chemical durability, and ease of processing, they are extensively used in glazing, packaging, containers, as well as materials intended for the construction sector. Their composition is mainly based on the (SiO_2-Na_2O-CaO) system, where silica acts as the glass network former, sodium oxide as the fluxing agent, and lime as the stabilizer [2].

Among the thermal properties of these materials, melting temperature occupies a central role due to its direct influence on manufacturing processes. In particular, it affects energy consumption, glass melt viscosity, melt homogeneity and, consequently, the industrial costs associated with glass production [3]. However, the experimental determination of this property remains complex and costly, especially when a large number of compositions must be investigated.

The melting temperature of glasses strongly depends on their chemical composition. Increasing the (SiO_2) content generally tends to strengthen the glass network and increase the melting temperature, whereas modifying oxides such as (Na_2O) promote its reduction through partial depolymerization of the silicate network [1] [2]. This complex interaction between the different oxides gives the system a highly nonlinear behavior, making the establishment of conventional predictive models difficult.

To overcome these limitations, artificial intelligence-based approaches have attracted increasing interest in the field of materials science. Among them, artificial neural networks (ANNs) stand out because of their ability to learn complex relationships between input and output variables from experimental data [4]. Several recent studies have demonstrated their effectiveness in predicting material and glass properties, particularly glass transition temperature, viscosity, and thermal properties [5] [6].

However, studies devoted to the prediction of the melting temperature of soda-lime glasses remain limited despite their industrial importance. In this context, the present study aims to develop an artificial neural network model capable of predicting the melting temperature of soda-lime glasses as a function of their chemical composition within the ternary (SiO_2-Na_2O-CaO) system. The objective is to evaluate the predictive performance of the model and assess its generalization capability through external and experimental validations.

2. Literature Review

2.1. General Overview of Glasses

Glass is an amorphous material obtained by cooling a molten liquid without sig-

nificant crystallization. Unlike crystalline materials, it does not exhibit long-range periodic order, which gives it particular properties such as transparency, chemical resistance, and the possibility of shaping at high temperatures [2].

According to Shelby [1], glass can be defined as "*a non-crystalline solid exhibiting the glass transition phenomenon*." Its structure is mainly composed of a three-dimensional network formed by interconnected polyhedral units.

Among the different existing glass families are silicate, borosilicate, phosphate, and chalcogenide glasses. Silicate glasses dominate industrial production (more than 90%) due to the abundance of silica resources and their technological properties [7] [8].

2.2. Soda-Lime Glasses: Composition and Structure

Soda-lime glasses constitute the most widely produced category of glasses worldwide, accounting for approximately 90% of industrial glass production [1]. They are used in glazing, bottles, containers, lamps, and construction applications.

Their typical composition includes [9]: SiO_2 (70% - 75%), which acts as the network former, Na_2O (13% - 17%) serving as the fluxing agent, and CaO (5% - 10%), which functions as a stabilizer.

Silica forms the structural backbone of glass through (SiO_4) tetrahedra. However, its high melting temperature (~1710˚C) makes its processing difficult [2].

The addition of sodium oxide induces depolymerization of the glass network through the breaking of oxygen bridges (*Si-O-Si*), thereby reducing viscosity and melting temperature [1].

Calcium plays a stabilizing role by improving the chemical durability and mechanical strength of the material [10].

2.3. Melting Temperature of Soda-Lime Glasses

Melting temperature corresponds to the temperature required to obtain a homogeneous liquid sufficiently fluid for industrial processing.

According to Seward and Vascott [3], controlling this temperature is essential because it influences:

- energy consumption;
- viscosity;
- melt homogeneity;
- industrial costs.

Soda-lime glasses generally melt between 1400˚C and 1600˚C, this range being strongly dependent on chemical composition [2].

Increasing the (SiO_2) content tends to increase the melting temperature due to the strengthening of the glass network. Conversely, fluxing agents such as (Na_2O) reduce this temperature by weakening the silicate structure [1].

Studies by Hong and Speyer [11] demonstrated that soda-lime glass synthesis involves several concurrent reaction pathways during melting, which explains the complexity of the associated thermal behavior.

2.4. Influence of Chemical Composition on the Thermal Properties of Glasses

The thermal properties of glasses are strongly governed by their chemical composition.

Oxides are generally classified into three categories [2]:

- Network formers: (SiO_2), (B_2O_3)
- Modifiers: (Na_2O), (K_2O)
- Intermediates/Stabilizers: (CaO), (MgO), (Al_2O_3)

The introduction of modifying oxides reduces the connectivity of the glass network and facilitates melting. In contrast, increasing the content of network-forming oxides generally increases viscosity and the characteristic temperatures of glass [12].

This nonlinear dependence between composition and properties makes the establishment of universal analytical equations difficult.

2.5. Modeling of Material Properties and Artificial Intelligence

Artificial intelligence is increasingly used in materials science to predict physical properties from experimental data.

Artificial neural networks (ANNs), inspired by the functioning of the human brain, are capable of learning complex relationships between variables [4].

This capability of ANNs to model highly nonlinear relationships has been exploited in several engineering fields for the prediction of complex physical properties, particularly in flow systems and transport phenomena [13].

A neural network consists of:

- an input layer;
- hidden layers;
- an output layer.

ANNs are particularly suitable for nonlinear systems where analytical models become insufficient.

According to Bishop [14], these methods improve predictive performance in complex systems involving multiple variables.

2.6. Applications of Neural Networks in Glass Science

Neural networks have already been used to predict several glass properties, including:

- viscosity;
- density;
- glass transition temperature;
- refractive index;
- optical properties.

However, studies specifically addressing the melting temperature of soda-lime glasses remain limited.

This limitation represents a scientific opportunity to develop predictive models

adapted to these glass systems.

Therefore, the present study proposes an ANN-based approach to establish a relationship between chemical composition and melting temperature.

3. Materials and Methods

Python programming language was used throughout this study for data preprocessing and normalization, implementation and training of the artificial neural network (ANN) model, as well as for the evaluation of predictive performance. The TensorFlow/Keras libraries were used to develop the neural network architecture, while the obtained results were analyzed using statistical indicators such as the coefficient of determination (R^2), the mean absolute error (MAE), and the root mean square error (RMSE).

3.1. Database and Studied Compositions

The study focused on the SiO_2-Na_2O-CaO ternary system, representative of soda-lime glasses commonly used in the glass industry. The data used were collected from both the literature and experimental measurements, covering a wide range of compositions in order to ensure the representativeness of the investigated compositional space.

The database used in this work consists of 45 compositions collected from six different literature sources. Among these compositions, 1 composition was extracted from Grynberg [15], 2 compositions from Bergeron and Risbud [16], 30 compositions from Zhang *et al.* [17], 3 compositions from Schairer [18], 3 compositions from Zhang *et al.* [19], and 6 compositions from Daud and Abu Hassan [20]. The experimental DSC endpoint temperatures reported by Zhang *et al.* [17] were considered as the melting temperatures for the corresponding compositions. Before training the ANN model, the collected data were carefully examined to remove duplicate and near-duplicate compositions. Compositions having identical SiO_2, Na_2O, and CaO molar fractions, or equivalent compositions after rounding, were considered duplicates, and only one representative composition was retained. Finally, 45 unique compositions were used for model development and validation.

Each input consisted of the molar fractions of SiO_2, Na_2O, and CaO, associated with the corresponding melting temperature.

3.2. Data Preprocessing

Before training, the data were normalized using the z-score method in order to reduce the impact of scale differences between variables [21].

The dataset was subsequently divided into two subsets:

- 80% for model training;
- 20% for evaluating the generalization capability.

The dataset was randomly divided into training and testing subsets using the train_test_split function from the Scikit-learn library. Eighty percent (80%) of the

data were used for model training, while the remaining twenty percent (20%) were reserved for testing the generalization capability of the model. The splitting process was performed randomly without stratification, and a fixed random seed (random_state = 44) was used to ensure reproducibility of the results.

Table 1 summarizes the molar fraction compositions of the mixtures in the SiO_2-Na_2O-CaO system, together with the corresponding melting temperatures used for the development and external validation of the model [15]-[20].

Table 1. Molar fraction compositions of the SiO_2-Na_2O-CaO mixtures.

N°	SiO_2	Na_2O	CaO	T (°C)	Type de mélange	N°	SiO_2	Na_2O	CaO	T (°C)	Type de mélange
1	0.000	1.000	0.000	1132	Pure	23	0.450	0.070	0.480	1325	Ternary
2	0.000	0.000	1.000	2570	Pure	24	0.460	0.080	0.460	1303	Ternary
3	0.330	0.000	0.670	2130	Binary	25	0.460	0.120	0.420	1300	Ternary
4	0.390	0.200	0.410	1428	Ternary	26	0.460	0.110	0.430	1315	Ternary
5	0.390	0.210	0.400	1425	Ternary	27	0.470	0.080	0.450	1325	Ternary
6	0.410	0.220	0.370	1315	Ternary	28	0.470	0.090	0.440	1317	Ternary
7	0.410	0.240	0.350	1292	Ternary	29	0.470	0.110	0.420	1285	Ternary
8	0.450	0.220	0.330	1300	Ternary	30	0.470	0.130	0.400	1305	Ternary
9	0.410	0.250	0.340	1300	Ternary	31	0.470	0.140	0.390	1310	Ternary
10	0.420	0.110	0.470	1325	Ternary	32	0.475	0.115	0.410	1287	Ternary
11	0.420	0.100	0.480	1320	Ternary	33	0.500	0.500	0.000	1400	Binary
12	0.420	0.250	0.330	1300	Ternary	34	0.500	0.000	0.500	1544	Binary
13	0.425	0.225	0.350	1300	Ternary	35	0.620	0.230	0.150	1450	Ternary
14	0.430	0.080	0.490	1325	Ternary	36	0.740	0.130	0.130	1450	Ternary
15	0.430	0.090	0.480	1320	Ternary	37	0.740	0.160	0.100	1450	Ternary
16	0.433	0.104	0.463	1305	Ternary	38	0.740	0.200	0.060	1450	Ternary
17	0.440	0.210	0.360	1295	Ternary	39	0.750	0.150	0.100	1500	Ternary
18	0.440	0.065	0.495	1330	Ternary	40	0.780	0.110	0.110	1450	Ternary
19	0.445	0.200	0.355	1310	Ternary	41	0.780	0.140	0.080	1450	Ternary
20	0.450	0.070	0.480	1305	Ternary	42	0.780	0.170	0.050	1450	Ternary
21	0.450	0.090	0.460	1310	Ternary	43	0.800	0.100	0.100	1500	Ternary
22	0.450	0.170	0.380	1317	Ternary	44	0.800	0.150	0.050	1500	Ternary
						45	1.000	0.000	0.000	1723	Pure

3.3. Development of the Artificial Neural Network (ANN) Model

The ANN model was implemented using TensorFlow/Keras [22]:

- Inputs: molar fractions of SiO_2, Na_2O, and CaO;

- Two hidden layers, each containing 10 neurons, with ReLU (Rectified Linear Unit) activation, recognized for its fast convergence capability [23];
- Output: predicted melting temperature.

The ANN architecture adopted in this study was a 3-10-10-1 fully connected feed-forward network. The input layer consisted of three neurons corresponding to the molar fractions of SiO_2, Na_2O, and CaO. Two hidden layers containing 10 neurons each were used with the Rectified Linear Unit (ReLU) activation function, while the output layer contained one neuron corresponding to the predicted melting temperature.

The model was trained using the Adam optimizer with the mean squared error (MSE) as the loss function, while the mean absolute error (MAE) was used as an additional evaluation metric. The training process was performed for 9500 epochs with a batch size of 32. A fixed epoch stopping criterion was adopted; training was stopped after 9500 epochs when the loss convergence became stable.

The 3-10-10-1 architecture was selected because the studied problem involves only three input variables and a limited dataset. The use of two hidden layers with 10 neurons provides sufficient nonlinear learning capacity while limiting the number of trainable parameters and reducing the risk of overfitting. The ReLU activation function was chosen because of its ability to efficiently model nonlinear relationships and improve convergence during neural network training.

3.4. Performance Evaluation

The model performance was evaluated using the coefficient of determination (R^2), MAE, and RMSE.

The choice of these metrics is justified by their relevance in materials property modeling [24].

The results were represented through:

- a loss convergence curve;
- correlations between experimental and predicted temperatures;
- ternary diagrams to visualize the compositional space.

4. Results and Discussion

The present study based on artificial neural networks (ANN) is a continuation of the work of Thio *et al.* [25], dedicated to the modeling of the liquidus of vitrifiable mixtures in the SiO_2-Na_2O-CaO system using a mathematical approach based on mixture planes.

4.1. Performance of the Artificial Neural Network Model

Thio *et al.* developed several polynomial models (first-order, second-order, third-order synergistic, and complete third-order models) to establish a relationship between the chemical composition and the melting temperature of vitrifiable mixtures. Among these models, the complete third-order model showed the best performance with a coefficient of determination of $R^2 = 0.9908$ [25].

In the present work, the ANN approach applied to the same ternary system (SiO_2-Na_2O-CaO) shows an improvement in predictive performance, with a coefficient of determination of R^2 = 0.9997 on the training dataset, associated with a MAE of 2.74˚C and an RMSE of 4.66˚C. This is illustrated in Figure 1 and Figure 2.

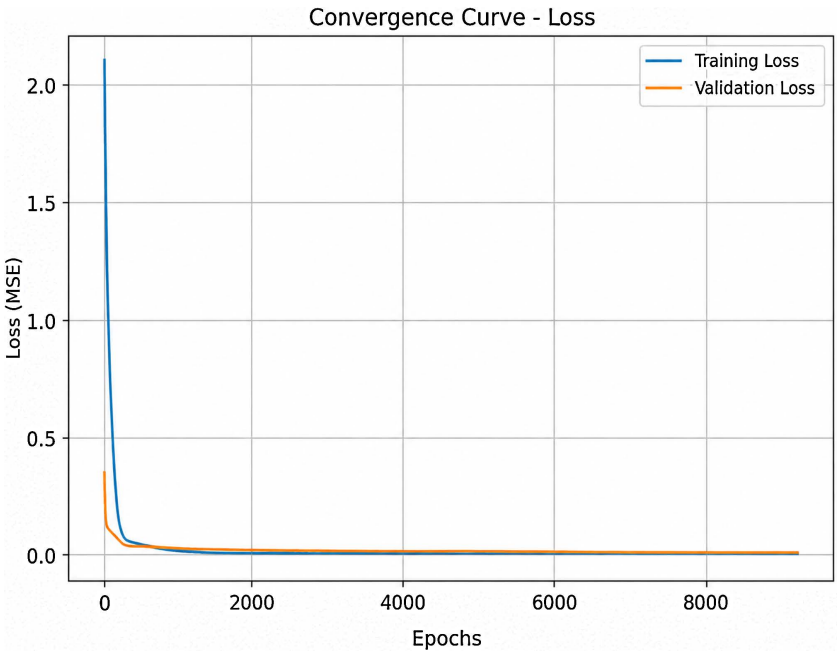

Figure 1. Loss convergence curve of the model.

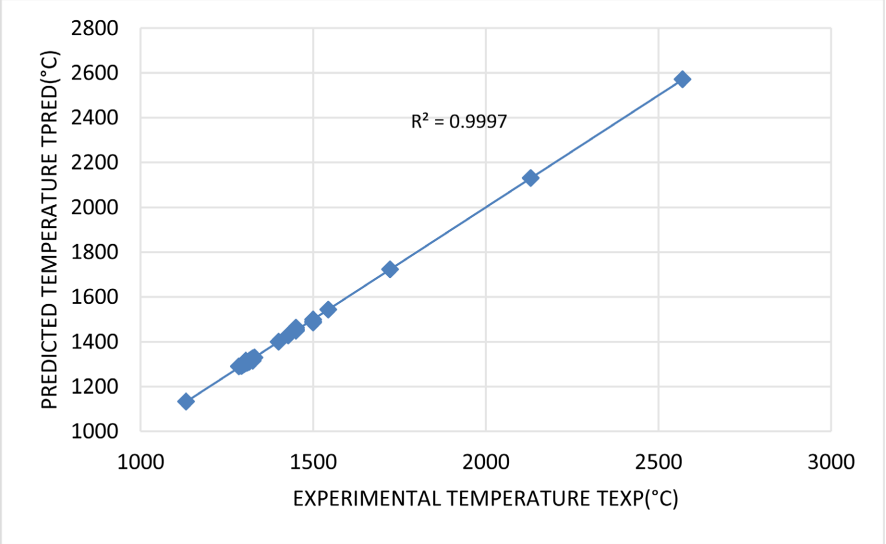

Figure 2. Correlation curve between predicted melting temperatures and experimental melting temperatures of the training dataset.

In Table 2, the difference between predicted and experimental temperatures highlights the predictive capability of the ANN model on the external validation dataset, with a coefficient of determination of R^2 = 0.9314, indicating that the

model explains 93.14% of the variability of the experimental temperatures from the external validation set.

Table 2. Molar composition of the external validation dataset.

N°	SiO_2	Na_2O	CaO	T_{EXP}	T_{PRED}	$\|T_{PRED} - T_{EXP}\|$
1	0.410	0.250	0.340	1300.00	1291.85	8.15
2	0.445	0.20	0.355	1310.00	1282.34	27.66
3	0.390	0.210	0.400	1425.00	1405.5	19.5
4	0.740	0.160	0.100	1450.00	1479.33	29.33
5	0.620	0.230	0.150	1450.00	1470.51	20.51
6	0.470	0.140	0.390	1310.00	1326.41	16.41
7	0.430	0.080	0.490	1325.00	1323.21	1.79
8	0.450	0.170	0.380	1317.00	1348.43	31.43
9	0.475	0.115	0.410	1287.00	1277.15	9.85

Although the errors slightly increased for the independent data, the obtained values (MAE = 18.29˚C and RMSE = 20.68˚C) remained moderate with respect to the investigated temperature range. These results therefore confirm the robustness of the model as well as its ability to generalize predictions beyond the training data.

This result indicates that the ANN captures the nonlinear relationship between oxide composition and melting temperature, in agreement with the performances reported by Ravinder *et al.* [5] for the prediction of glass transition temperatures and by Cassar *et al.* [26] for thermal properties related to the melting behavior of functional glasses.

These results confirm the robustness of the adopted approach and the relevance of neural networks for modeling complex thermophysical properties.

The slight decrease in performance between training and external validation suggests the onset of overfitting, a phenomenon commonly observed with limited datasets. However, an R^2 value greater than 0.90, as shown in **Figure 3**, remains a strong indicator in the field of materials property prediction [24].

Although the developed ANN model demonstrated high predictive performance, some limitations should be highlighted. The relatively small size of the dataset (45 compositions) may restrict the generalization capability of the model, particularly for compositions located outside the investigated SiO_2-Na_2O-CaO compositional domain. Moreover, the decrease in performance observed between the training stage and external validation indicates that the robustness of the model should be interpreted with caution. Therefore, further enrichment of the database with additional experimental compositions will be necessary to improve extrapolation capability and confirm the reliability of the proposed approach.

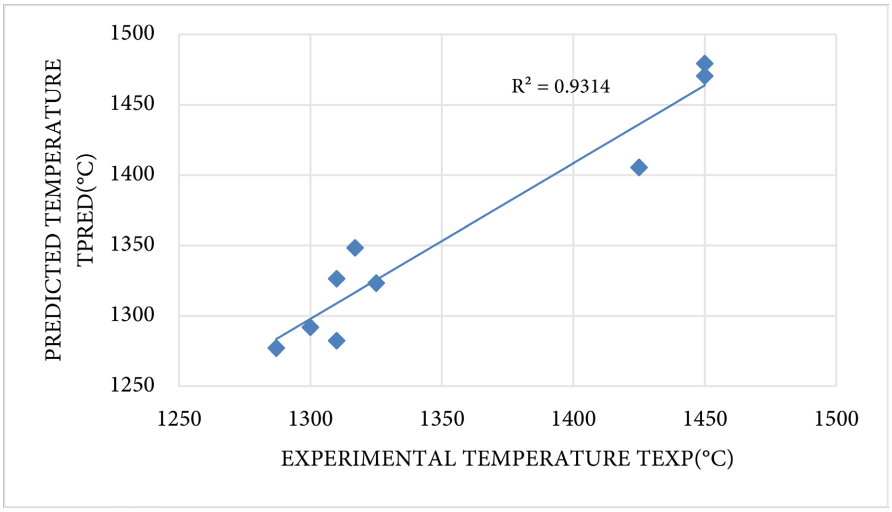

Figure 3. Correlation curve between predicted melting temperatures and experimental melting temperatures of the external validation dataset.

4.2. Ternary Diagrams and Qualitative Validation

The comparison between the ternary diagram generated by the ANN model (**Figure 4**) and that constructed from experimental data (**Figure 5**) highlights the correspondence between the predicted and measured melting domains in the SiO_2-Na_2O-CaO system.

This visual and structural agreement is particularly significant, as it shows that the model is not only capable of reproducing individual numerical values with accuracy ($R^2 > 0.93$), but also of restoring the overall topology of the compositional space.

This capability to model global trends is consistent with the observations reported by Cassar *et al.* [27], who demonstrated that AI-evolutionary algorithm approaches can reproduce property maps close to experimental reality.

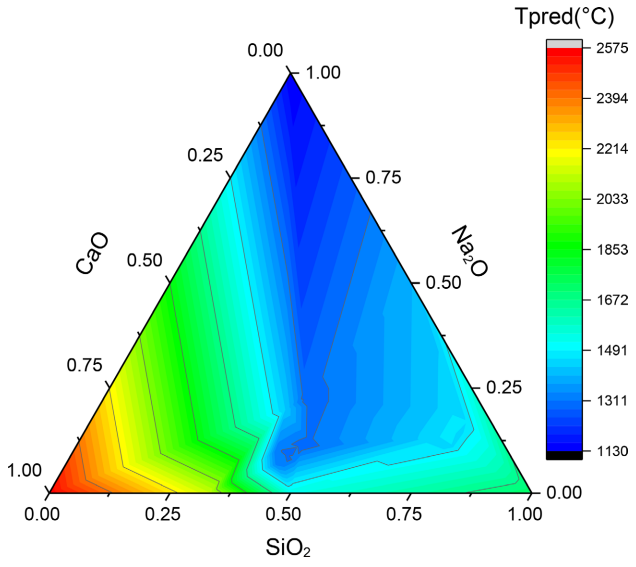

Figure 4. Ternary diagram of the SiO_2-Na_2O-CaO ternary system generated by the model.

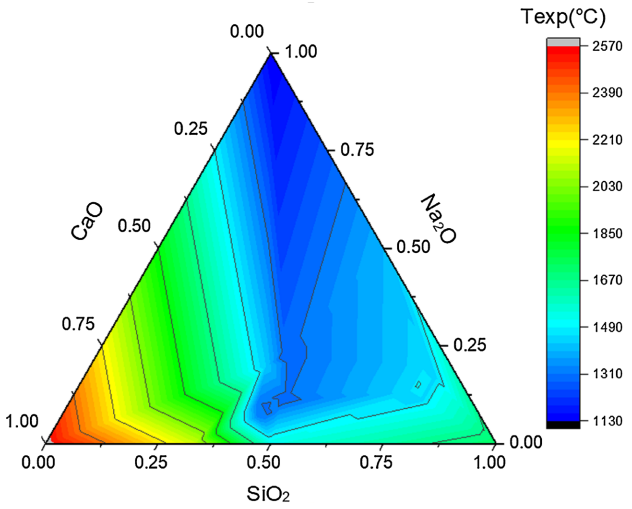

Figure 5. Ternary diagram of the SiO_2-Na_2O-CaO system derived from experimental data.

This strengthens the credibility of using ANN models for the exploration of new glass compositions while reducing the dependence on extensive experimental campaigns.

4.3. Experimental Validation of the Model Using Experimental Data

To further evaluate the predictive capability of the developed artificial neural network (ANN), an additional experimental validation was carried out using independent data reported by Santoso *et al.* [28]. The selected compositions belong to the SiO_2-Na_2O-CaO ternary system and were not included in the database used for training or external validation of the model. These data, obtained from independent equilibrium experiments, provide a relevant case study for assessing the predictive performance of the model on compositions that were not used during its development.

The comparison between the experimentally reported melting temperatures and those predicted by the ANN model is presented in **Table 3**. The obtained results show that the model provides satisfactory predictions over the investigated compositional domain. Most of the prediction errors remain limited, indicating that the ANN successfully captures the nonlinear relationship between chemical composition and melting temperature. Larger deviations are observed for some compositions, particularly at higher melting temperatures, which may be attributed to the increased complexity of phase equilibria in these compositional regions and to the limited number of experimental data available for training.

The calculated performance indicators further confirm the predictive capability of the proposed model. The Mean Absolute Error (MAE) and the Root Mean Square Error (RMSE) were found to be 14.35˚C and 19.12˚C, respectively. Considering that the investigated melting temperatures cover a range of approximately 1300˚C - 1400˚C, these errors remain relatively small and demonstrate that the ANN model provides reliable temperature estimations for independent exper-

imental compositions.

Table 3. Experimental validation of the ANN model using independent compositions reported by Santoso *et al.* [28].

N°	SiO_2	Na_2O	CaO	T_{EXP}	T_{PRED}	$\lvert T_{PRED} - T_{EXP} \rvert$
1	0.450	0.117	0.433	1300	1297.68	2.32
2	0.454	0.079	0.467	1300	1309.56	9.56
3	0.418	0.264	0.318	1300	1296.83	3.17
4	0.755	0.054	0.191	1400	1433.75	33.75
5	0.422	0.168	0.410	1400	1429.89	29.89
6	0.425	0.142	0.433	1400	1407.41	7.41

Overall, this additional validation confirms the robustness of the developed model and highlights its potential as a practical tool for estimating the melting temperature of soda-lime glasses from their chemical composition. Such predictive capability can considerably reduce the number of experimental trials required during glass formulation and facilitate the preliminary design of new vitrifiable compositions.

5. Conclusions

This study led to the development of an artificial neural network (ANN) model for the modeling and prediction of the melting temperature of soda-lime glasses in the ternary (SiO_2-Na_2O-CaO) system based on their chemical composition. The proposed approach relies on the use of the molar fractions of the main glass-forming oxides as input variables and the melting temperature as the output variable.

The obtained results highlighted the predictive capability of the developed model. On the training dataset, the network achieved a coefficient of determination of $R^2 = 0.9997$, associated with a Mean Absolute Error (MAE) of 2.74˚C and a Root Mean Square Error (RMSE) of 4.66˚C, indicating that the predicted temperatures are close to the experimental temperatures.

External validation confirmed the robustness of the model with a coefficient of determination of $R^2 = 0.9314$. Furthermore, experimental validation yielded a MAE of 14.35˚C and an RMSE of 19.12˚C, supporting the model's ability to generalize to compositions not included in the training dataset.

Furthermore, the comparison between the experimental ternary diagrams and those generated by the ANN model revealed an interesting reproduction of the global trends of the compositional system, demonstrating the capability of the network to reproduce not only individual values but also the organization of the compositional space of soda-lime glasses.

Overall, these results confirm the relevance of artificial neural networks as a predictive tool for the thermal properties of glassy materials. This approach represents a promising alternative to conventional experimental methods by reduc-

ing the time, costs, and number of tests required for the exploration of glass compositions.

As perspectives, this approach could be extended to more complex glass systems and coupled with optimization methods for the identification of new low-melting compositions.

Furthermore, this model could be used in future glass paste production experiments, where it would serve as a predictive guide for the identification and selection of vitrifiable soda-lime mixtures. Thus, the developed model could serve as a formulation support tool by guiding experimental investigations toward composition domains favorable to vitrification and the development of new glass pastes suitable for technological and artistic applications.

Author Contributions

Mohamed KARAMOKO: Conceptualization, Data curation, Methodology, Software, Formal analysis, Validation, Visualization, Writing—original draft.

Peyokoh Roger THIO: Conceptualization, Data curation, Methodology, Writing—review and editing.

Kouassi Bruno KOFFI: Supervision, Investigation, Methodology, Validation, Writing—review and editing.

Kouadio Denis KONAN: Project administration, Writing—review and editing.

All authors have read and agreed to the published version of the manuscript.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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