THE POSSIBILITY OF MODELING AGRICULTURAL BIOMASS ASH BY NEURAL NETWORKS CONCERNING PROXIMATE ANALYSIS INPUTS

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Agricultural biomass is an important renewable energy source with significant environmental and economic benefits. However, high ash content in biomass can lead to problems such as slagging, fouling, and corrosion and can reduce the efficiency of energy systems. This study analyzes the proximate composition of different biomass samples, focusing on ash content, and uses machine learning to model ash content based on other components. Six biomass types, including rapeseed, barley, wheat, corn, soybean and sunflower, were examined to analyze the content of coke, fixed carbon (FC), volatile matter (VM) and ash. The results showed considerable variability, with ash content ranging from 8.25 % for rapeseed to 12.3 % for soybean. Artificial neural networks (ANN) were used to model ash content with a high accuracy of R^2 = 0.92. The model effectively estimated the ash content based on the input parameters and demonstrated the potential of machine learning to optimize biomass selection for energy production.

Key words: *biomass, artificial neural networks, proximate analysis, ash content, modelling.*

1. Introduction

Biomass has attracted considerable attention as a key renewable energy source that can play a crucial role in reducing dependence on fossil fuels and mitigating climate change. Biomass refers to organic materials such as agricultural residues, forestry by-products, and specialized energy crops that can be converted into bioenergy through various processes such as combustion, gasification, and anaerobic digestion [1]. The use of biomass to generate energy not only offers a sustainable alternative to conventional fuels but also promotes the circular economy by valorizing waste materials. Biomass is considered carbon neutral as the CO_2 released during combustion is offset by the CO_2 absorbed during the growth of the biomass [2].

The European Union (EU) has set ambitious targets for renewable energies as part of its climate and energy policy. The Renewable Energy Directive (RED II) [3], which is part of the European Green Deal, advises that at least 32% of energy consumption in the EU should come from renewable sources by 2030 Mehedintu et al., (2021) [4]. Biomass is expected to play an important role in achieving these targets due to its versatility and availability. The EU's focus on sustainability has led to strict criteria for the sourcing of biomass to ensure that biomass production does not endanger food security and biodiversity [5]. These criteria are designed to promote sustainable land management practices and protect natural ecosystems while maximizing the climate benefits of biomass.

Despite its advantages, the use of biomass for energy production poses certain challenges, particularly about its ash content [6]. Ash as an inorganic residue that remains after the complete combustion of biomass contains minerals such as silica, alumina, iron oxide, and various alkali metals [7,8]. A high ash content can lead to various operational problems in biomass energy systems, e.g. slag deposits and metal corrosion in combustion systems [9]. The management and disposal of ash residues also require careful handling and can be associated with additional costs. Considering the critical influence of ash content on biomass utilization, this study aims to perform a detailed analysis of the proximate composition of different biomass samples with a focus on ash content. By examining parameters such as coke, fixed carbon (FC), volatile matter (VM), and ash, we seek to identify biomass types with favorable characteristics for energy production. VM, ash content, and FC content are important components for characterizing fuel materials. Biomass having high volatile matter and low ash content is generally a promising feedstock for biofuel production [10].

Rapeseed and sunflowers are characterized by a low to moderate ash content and good combustion properties, making them suitable for efficient bioenergy applications. Although barley and wheat have a higher ash content, they offer a high fixed carbon content, reflected in a high energy yield. Corn, characterized by a high content of volatile components, is ideal for pyrolysis and gasification. Despite the higher ash content, soy provides a high energy yield due to high fixed carbon content.. These diverse biomass sources, which are abundant in agricultural residues, underline the potential for optimized and sustainable bioenergy production.

Machine learning models have recently been increasingly used for modeling and estimation purposes in various fields of engineering [11]. Machine learning algorithms enable modeling with big data to achieve task-specific results and modeling of outcomes [12]. For such tasks, MLP (Multi Layer Perceptron) ANNs, which take the approach of selecting a set of dependent variables and thus creating predictive models for these variables, have proven to be one of the most suitable forms [13]. Conventional methods of mathematical models for estimating desired output values cannot fully capture the nonlinearity present in the data, thus artificial neural network (ANN) models appear as an applicable high-performance tool [14]. ANN models have self-learning capabilities and can be described as a system consisting of units (artificial neurons) connected into a single unit that forms a network [15]. The main challenges in applying machine learning in research include missing (quality) data and missing annotations, which limits the reliability of the model. In addition, larger computational resources are usually required for efficient model training. Furthermore, it is important to point out that such models often face challenges when it comes to integrating them between different systems and ensuring their comprehensibility and usability [16]. Ramachandra and Mandal, (2023) [17] conducted a study to predict the ash content in different types of concrete using ANN and SVM (Support Vector Machine) algorithms. A total of 406 data points were used for the study and they achieved high accuracy in terms of correlation coefficient for ANN (0.97) and SVM (0.98). The SVM model performed better with lower MAE and RMSE values. On the other hand, Abhishek et al., (2023) [18] developed an ANN model to estimate the compressive strength of concrete with corn cob ash. The model had an average accuracy of 98%, which shows that ANN is an effective method for estimation in the mentioned applications.

The aim of this research was to develop an artificial neural network (ANN) for the prediction of ash content in different types of biomass based on input variables such as the content of coke, fixed carbon (FC) and volatile matter (VM). The research is focused on accurate ash modeling using machine learning, to optimize the biomass selection processANN is used to improve the accuracy of these predictions, providing a valuable tool for biomass selection and processing optimization. These models have been trained and validated using compositional data from different biomass samples, demonstrating their potential to predict ash content with high accuracy.

2. Materials and Methods

2.1. Feedstock selection and collection

Six biomass of post-harvest residues were characterized in this study, three oilseeds: rapeseed, soybean and sunflower and three cereals: wheat, barley, and corn. All examples that have been collected are first dried at 60 °C to remove moisture. After drying, the sample was ground using a crasser machine and rubbed using a flouring device until it reached 500 μm.

2.2. Proximate analysis of biomass

Proximate analysis was conducted on biomass materials to determine ash content (AC), volatile matter (VM), and fixed carbon (FC). All analyses were carried out in triplicate, and the average values were reported.

2.3. Determination of ash content, volatile matter, and fixed carbon

0.5–1 g of each biomass sample is weighed into pre-dried porcelain pots in a laboratory dryer at 105 °C for 1 h. Subsequently, the samples are placed in the muffle furnace, Naberthertm GmbH at a temperature of 550 °C for 5h30min with an initial preheating time of 15 min. After cooling to room temperature, the ash content is determined by calculating the difference in sample weight before and after the procedure. Volatile matter comprises the compounds that vaporize when the biomass is heated, influencing combustion characteristics. In this study, the ash content was determined by heating the sample in an inert atmosphere at 900 °C for 4 minutes and then calculating the weight loss without moisture. Fixed carbon is the solid combustible residue left after the release of volatile matter, indicating the potential energy content. This parameter was calculated indirectly as the difference between 100% and the sum of moisture, ash, and volatile matter percentages. The coke content was determined by burning the biomass sample in a muffle furnace at a temperature of 900 °C for 5 minutes. After combustion, the samples were placed in a desiccator to cool down. The coke content was calculated based on the mass difference before and after combustion.

2.4. Statistical analysis

After the laboratory analysis, the data was compiled in Excel and a database was created in .csv format. The data was statistically processed to determine descriptive statistics. To determine the differences between the observed categories, an analysis of variance (ANOVA) and the LSD test (Fisher Least Significant Difference) were performed. To assess the degree of correlation between the variables studied in the research, a correlation analysis was also performed and the distribution of each variable in relation to the category of the sample was presented. All statistical analyzes were performed in the Python programming language [14] using the coresponding packages.

2.5. Artificial neural networks (ANN)

To create a database for the modeling, a total of 521 samples were used, which were categorized according to the type of biomass. When creating the model, different types of biomass were categorized and processed using the one-hot encoding method. This method converted the biomass types into separate binary attributes, which enabled the correct integration of categorical data [19]. The architecture of the developed model is sequential, with each layer receiving input values from the previous layer. During the development of the ANN model, a hyperparametric optimization was performed to find the optimal settings for the neural network. Different combinations of hyperparameters (number of layers (3-10), number of neurons per layer (1-20), and batch size (1-10)) were tested using grid search and random search methods.. The model was developed with a total architecture of 5 dense layers: 64 neurons in the first layer, 32 in the second and third layers, 16 in the fourth layer and 1 in the output layer (Fig 1). The activation functions used are Rectified Linear Unit (ReLU) for the first four layers, which provide nonlinearity [20], while a linear function is used for the output layer, which in this case is suitable for a regressive task. The ADAM algorithm [21] was used to optimize the model, which has high performance in updating the weighting coefficients with respect to data loss. The chosen architecture of the ANN model, which consists of 5 dense layers and a certain number of neurons, was obtained through an iterative process of trial and error methods. In this process, different architectures were tested and evaluated, with the final configuration selected based on the best performance of the model in terms of prediction accuracy and generalization on validation data. The model was trained with 4000 epochs (number of iterations in the learning process), corresponding to the total number of runs through the entire training dataset. The batch size was set to 50, which affects the training speed and convergence stability of the model. The modeling data is randomly divided into two parts, a learning

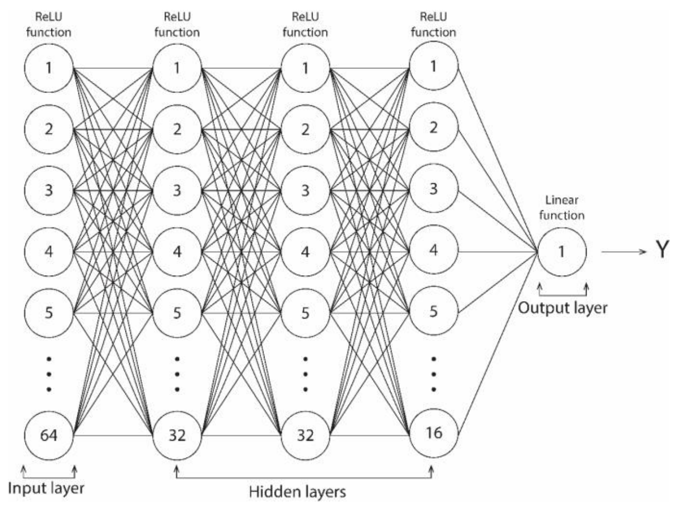

Figure 1. Schematic representation of the ANN model developed for estimating the ash content as a function of the input data of the proximate analysis

part (80%) and a validation part (20%). This data split allowed the model to learn from a larger data set while validating the model with a smaller data set to determine the possibility of generalizing an unseen portion of the data[22]. The ANN model was used to create the Python programming language with the associated packages (pandas, seaborn, NumPy and Tensorflow).

2.6. Model evaluation

Once the ANN model had been created and the calculations obtained, a statistical analysis was carried out to evaluate the model. For this purpose, the error metrics Root Mean Squared Error (RMSE) (1), Mean Absolute Error (MAE)(2), Mean Biased Error (MBE) (3), and Mean Percentage Error (MPE) (4) were used. To show the degree of regression achieved by the model, the coefficient of determination (R^2) (5) was also used as a benchmark [23,24]:

$$RMSE=\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_t-y_p)^2} \tag{1}$$

$$MAE=\frac{1}{n}\sum_{i=1}^{n}\left|y_t-y_p\right| \tag{2}$$

$$MBE=\frac{1}{n}\cdot\sum_{i=1}^{n}(y_p-y_t) \tag{3}$$

$$MPE=\frac{100}{n}\cdot\sum_{i=1}^{n}\left(\frac{\left|y_p-y_t\right|}{\left|y_t\right|}\right) \tag{4}$$

$$R^2=1-\frac{\sum_{i=1}^{n}\left(y_p-y_t\right)^2}{\sum_{i=1}^{n}(y_p-y^m)^2},\ y^m=\frac{\sum_{i=1}^{n}y_t}{n} \tag{5}$$

Where y_p are the values determined by the model and y_t are the target values

3. Results

Tab. 1 shows a proximate analysis of the biomass of different agricultural crops, including rapeseed, barley, wheat, corn, soybean, and sunflower.

Tab. 1 provides a detailed comparative analysis of the proximate composition with parameters coke, fixed carbon (FC), volatile matter (VM), and ash content. The highest coke content was observed in wheat (26.90 %), while corn exhibited the lowest coke content (16.21%). Barley had the highest FC content (16.42 %) while corn had the lowest FC content (6.27 %). VM content was highest in corn (75.66 %) and lowest in barley (65.96 %). The ash content was highest in soy (12.30 %) and lowest in rapeseed (8.25 %).

Table 1. Statistical analysis of proximate composition in various biomass samples

Sample	Coke (%)	FC (%)	VM (%)	Ash (%)	MC (%)
Rapeseed	17.94± 2.71^{AB}	9.64± 2.12^{A}	72.24± 2.59^{B}	8.25± 1.31^{A}	7.44± 2.66^{AB}
Barley	26.62± 18.56^{C}	16.42± 17.3^{B}	65.96± 17.27^{A}	10.54± 3.91^{BC}	7.03± 2.79^{AB}
Wheat	26.9± 19.94^{C}	15.23± 19.11^{B}	65.97± 18.31^{A}	11.67± 3.57^{CD}	9.63± 1.44^{C}
Corn	16.21± 2.89^{AB}	6.27± 3.57^{A}	75.66± 3.49^{B}	9.92± 3.3^{B}	7.92± 1.56^{B}
Soy	21.45± 6.16^{B}	9.12± 3.98^{A}	71.82± 5.57^{B}	12.3± 4.64^{D}	10.83± 3.61^{D}
Sunflower	20.26± 4.65^{AB}	9.47± 2.79^{A}	71.62± 7.05^{B}	10.9± 3.51^{C}	6.7± 1.09^{A}
Minimum	16.21	6.27	65.96	8.25	6.70
Maximum	26.90	16.42	75.66	12.30	10.83
Average	21.57	11.02	70.54	10.60	8.26
CV	42.43	73.88	12.82	31.83	26.53
Statistical significance	*	*	*	*	*
MS	1675.7	1331.92	1284	164.56	41.67

Note: The results in the tab. 1 are given as mean values ± standard deviation; All results are presented on a dry basis. CV - Coefficient of Variation; MS – Mean square. Different letters in the same column represent the difference between the observed values according to the Fisher LSD post hoc test (*p < 0.05). Statistical significance: * p<0.01.

Fig. 2 shows the distribution of the investigated variables about the type of biomass (indicated by a different color) as a scatter plot with Pearson's correlation coefficient (r), with statistically significant correlations at p≤0.01 marked with asterisks (*).

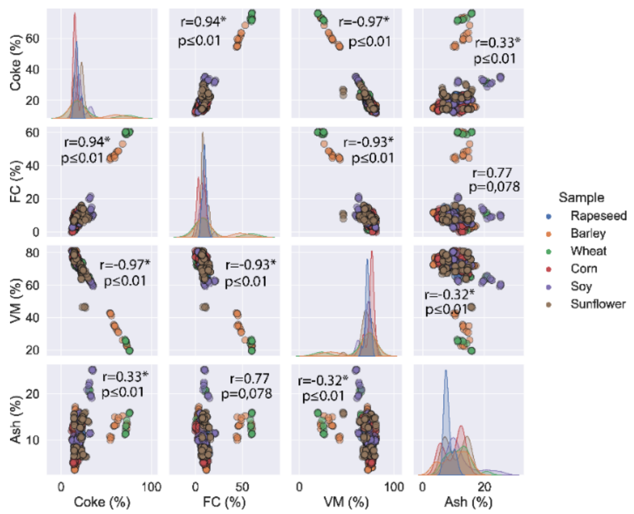

Figure 2. Correlation matrix of proximate composition parameters in various biomass samples

The variable ash (which was used as the initial variable of the ANN model) is positively correlated with FC (r=0.77) but does not show a statistically significant relationship. On the other hand, coke and ash are statistically significantly correlated at p≤0.01 (r=0.33), while VM and ash are negatively correlated (r=-0.32).

Fig. 3 shows the training and validation loss over an epoch in the process of modeling the ash content considering the inputs of the proximate analysis.

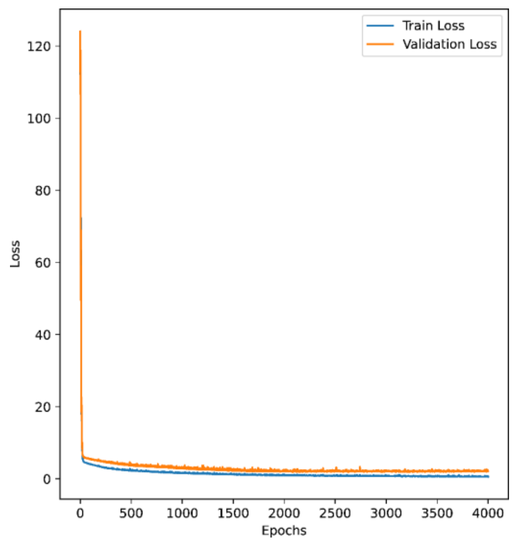

Figure 3. Training and validation loss over epochs

Both training and validation loss start at a high value, rapidly decreasing within the first few hundred epochs. As the number of epochs increases, the losses continue to decrease and stabilize, showing minimal fluctuations after around 1000 epochs.

Table 2. Statistical performance indicators of the developed ANN model for ash estimation

R^2	Train	0.93
	Test	0.88
	Overall	0.92
RMSE	Train	0.94
	Test	1.37
	Overall	1.04
MAE	Train	0.49
	Test	0.84
	Overall	0.56
MBE	Train	0.18
	Test	0.23
	Overall	0.19
MPE (%)	Train	2.42
	Test	4.08
	Overall	2.75
Execution time (s)		383

R^2 – Coefficient of determination; RMSE – Root mean squared error; MAE – Mean absolute error; MBE - Mean biased error; MPE – Mean percentage error

Tab. 2 shows the statistical performance indicators of the developed ANN model. The following metrics were used as error measures: RMSE, MAE, MBE and MPE. On the other hand, R^2 is used as a specific indicator of the regression of the model.

ANN showed high performance in modeling the ash content (Tab. 2). The overall R^2 value was 0.92, indicating that the model has a high degree of regression, which can also be seen in Fig. 4. When looking at the modeling error, all statistical indicators have a low error level.

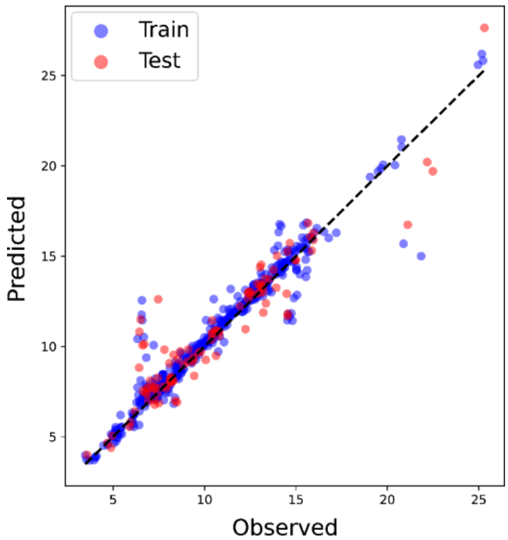

Figure 4. Scatter plot of the observed versus the predicted ash content using the ANN model

4. Discussion

Proximate analysis of the six biomass samples analyzed in this study revealed considerable variability in their composition. Rapeseed biomass sample demonstrated relatively low ash content

(8.25%) compared to other types of biomass and high volatile matter (72.24%). Tahir et al. (2019) [25] reported a higher VM of 81.85% and a significantly lower ash content of 4.83% for rapeseed biomass. The above-mentioned variability is possible due to different cultivation and climatic conditions. Barley showed the highest coke (26.624%) and FC (16.42%) content among the samples, with an ash content of 10.54% and VM of 65.96 %. Despite the higher ash content, barley's substantial FC suggests a high energy yield, though ash management strategies are necessary. Wheat biomass exhibited a high ash content (11.67%) and comparable FC (15.23%) and VM (65.97%) levels. Shen et al. (2010) [26] reported FC values for wheat straw ranging from 18.95% to 23.50%, VM from 63.00% to 71.78%, and ash content from 9.27% to 13.50%, indicating that our results fall within these reported ranges. The higher ash content poses challenges but can be mitigated with appropriate combustion technologies.

Corn biomass had the lowest coke (16.214%) and a high VM (75.66%), with moderate ash content (9.92%). These values differ from those reported by Sulaiman (2019) [27], who found VM of 55%, FC of 44.3%, and ash content of 0.7% in corn stalks. Soy biomass displayed a relatively high ash content (12.3%) and FC of 9.12%. Motghare et al. (2016) [28] reported lower values for soybean waste, with an ash content of 4.7%, VM of 70.5%, and FC of 19.0%. This indicates that the composition of soybean biomass can vary significantly. The higher ash content in this research findings suggests greater challenges in combustion processes compared to the lower ash content reported by Motghare et al. (2016) [28]. Sunflower biomass showed moderate ash content (10.9%) and high VM (71.62%). These findings differ from those of Kułażyński (2018) [29] and Casoni (2019) [30], who reported lower ash contents (1.95% and 2.1%, respectively) and similar VM levels (77.72% and 79.8%). The moderate ash content and high volatile matter content suggest that sunflower biomass can be efficiently utilized for energy production with appropriate combustion technology.

The last part of the research involved the development of an ANN model to evaluate the possibility of its use in modeling the ash content of different types of biomass with respect to the input variables of the proximate analysis. Ash is an important indicator of fuel quality for which numerous assessment studies have been conducted [31-33]. The ANN model was developed in the sequential form of the architecture of 64-32-32-16 artificial neurons for the input, 2 hidden and output layers. The model showed high performance in ash estimation, as indicated by a high R^2 = 0.92 and low error levels RMSE (1.04), MAE (0.56), MBE (0.19) and MPE (2.75%). In comparison to the literature, (Ghosh et al., 2016) conducted a study in which he estimated ash based on the input variables of the geophysical log and core analysis data and achieved an R^2 of 0.84. To estimate the proportion of ash produced by burning coal in a power plant, Bekat et al., (2012) [34] used the ANN model using the input data of MC, ash content and LHV of the raw materials and obtained an R^2 >0.97. In addition, for the ANN model, I measured the execution time of the code, and the results were obtained after 383 seconds. ANN models of the regression type are subject to several limitations that have been analyzed in different studies. One of the most important limitations is the problem of sensitivity to the size of targets, where the MSE is unfavorable as a statistical measure for targets with different sizes, which can be solved by alternative methods such as loss histograms. Other research indicates that ANN models use non-linear algorithms that improve short-term predictions but not necessarily accuracy, so a combination with traditional statistical methods is required for better results [35]. In addition, ANN models often ignore specific laws in engineering applications, which can lead to inconsistent results [36]. It can be concluded that by combining different approaches, it is possible to overcome the main limitations of ANN regression models and improve their perfor-mance. Future research should focus on expanding the database for ash content modelling as well as expanding the categorical variables – in this case, biomass types. Also, in addition to the ANN model, future research should compare different approaches for machine learning regression models to determine the most appropriate model through comparison.

5. Conclusions

In summary, ANN models have potential for estimating the ash content in biomass and provide accurate predictions that can be used to optimize the selection of biomass for energy purposes. The main results of the research are:

- ANN models were trained on six types of biomass (rapeseed, barley, wheat, corn, soybean, sunflower) and showed high accuracy in estimating ash content with R^2=0.92
- Optimal hyperparameter values were determined using grid search and random search methods, and the Adam algorithm were used for model optimization.
- The results showed low error values: RMSE (1.04), MAE (0.56), MBE (0.19) and MPE (2.75%).
- ANN models recognize complex nonlinear relationships between the input variables and enable more accurate predictions compared to conventional linear regression models.
- One of the biggest challenges remains the need for large amounts of quality data for model training.
- The study showed considerable variability in ash content between different biomass types, which emphasizes the importance of adapted models for different biomass types.
- The combination of different approaches can further improve the accuracy and robustness of ANN models and make them a valuable tool in the field of renewable energy.

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