Smoke point prediction using ANN

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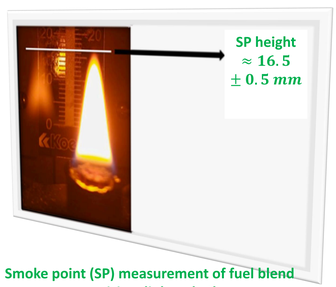
Figure 2: Distribution of some pure chemicals' functional groups

Introduction

Evaluating the sooting propensities of various fuels is necessary in order to reduce the emissions of pollutants like particulate matter (PM) from the engines. The smoke point (SP), which provides a numerical measurement of the fuel's sooting propensity, is frequently used as an index for this purpose. In this study, an artificial neural network (ANN) tool was used to develop a machine learning-based model based on experimental data of the measured smoke point of fuels comprising alcohol and ethers (121 pure compounds and 236 mixtures). One output and ten inputs make up the ANN model. The composition of fuels is expressed by eight inputs expressed by functional groups: paraffinic CH_3, paraffinic CH_2, paraffinic CH, naphthenic CH-CH_2, olefinic -CH=CH_2, aromatic C-CH, alcohol OH, and ether O groups. The molecular structure is represented by the two final inputs, molecular weight (MW) and branching index (BI). The measured smoke point is the output. 70% of the data were used to train the model, 15% were used to validate it, and 15% were used to test it. The developed model successfully explains the relationship between the experimental and predicted smoke points, with an R^2 correlation factor of 0.97. The predicted SP's mean absolute error was 4.5. The findings demonstrate that the aforementioned inputs are necessary for the created model to accurately predict SPs of fuels. So, provided the 10 inputs are known, this model may be used to forecast the SPs of the fuels (pure or mixed). Finally, alcohols or ethers can be added to the scanned fuels in accordance with the expected smoke point of those fuels in order to perhaps reduce the amount of particulate matter released (PM).



Smoke point (SP) measurement of fuel blend comprising diphenyl ether (20%) and diesel (80%) by volume.

Methodology

The functional groups (paraffinic CH_3, paraffinic CH_2, paraffinic CH, naphthenic CH-CH_2, olefinic -CH=CH_2, aromatic C-CH, alcohol OH, and ether O), as well as branching index (BI) and molecular structure (MW) of oxygenated fuels containing alcohols or ethers, have been used as 10 inputs for developing an artificial neural network (ANN) model. The calculations for the inputs are as follows: Using n-heptane(its structure is shown in figure 1) as an example, which has a molecular weight of 100 g/mole and is composed of seven groups, the paraffinic CH_3 and CH_2 groups account for 30 and 70 weight percent (wt.%) of the total weight of n-heptane, respectively. There are two CH_3 groups and five CH_2 groups. The remaining functional groupings have 0 weight percentages. The distribution of the functional groups of some (a) pure compounds and (b) mixtures ((A) 5% methylnaphthalene + 95% iso-octane, (B) Je t - A (47.06% n -dodecane + 16.69% iso -cetane + 24.19% decalin n + 12.06% toluene), (C) 11.5% tripropylene glycol methyl ether + 38. is displayed in figures 2(a) and 3(b), respectively, that follow. The branching index (BI), which numerically measures the size and position of methyl/methylene branches, is zero for n-heptane. As of right now, the measured smoke point (SP) and the estimated features (CH_3, CH_2, CH, naphthenic CH-CH_2, olefinic -CH=CH_2, aromatic C-CH, alcohol OH, ether O, BI, MW) can be used as an output and 10 inputs, respectively, for creating the ANN model. The general architecture of an artificial neural network (ANN) is shown in figure 4.

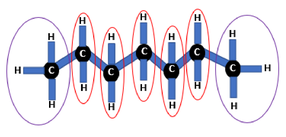


Figure 1: n-Heptane structure

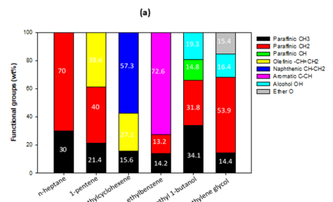


Figure 2: Distribution of some pure chemicals' functional groups

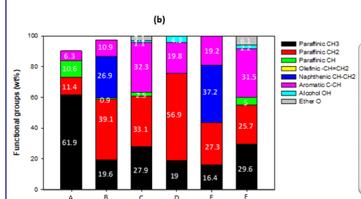


Figure 3: Distribution of the functional groups in some mixtures

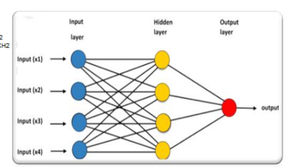


Figure 4: A conceptual representation of an artificial neural network

Results

Since most relationships between SPs and the ten characteristics of oxygenated fuels are nonlinear(e.g., as shown in Figure 5), the original and predicted smoke points have a poor correlation value (R^2 = 0.84) when the multiple linear regression(MLR) method is used. In other words, the last technique cannot properly capture all of the trends (correlations or linkages) among the smoke points and the specified functional groups, MW and BI, because they are nonlinear, as previously described. Hence, a trustworthy technique, such as those found in artificial intelligence or machine learning(e.g., an artificial neural network tool (ANN)), is needed for identifying all the aforementioned tendencies. The ANN was initially trained and validated concurrently, and then tested by 70, 15, and 15% of the data, respectively. The final optimized ANN parameters(shown in Table 1), which were one hidden layer, 10 neurons, and 317 epochs, are displayed in Figure 6. The R^2(0.97) correlation between experimental and predicted SPs is shown in Figure 7. This result highlights the significant difference between the old method (MLR), where R^2 is roughly 0.84, and the current method (ANN), where R^2 is nearly 0.97. The average absolute error, as shown in Figure 8, was about 4.5.

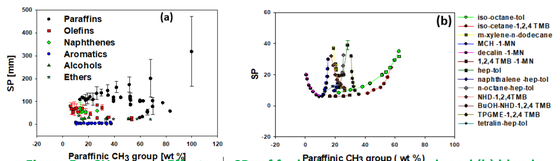


Figure 5:: CH_3 groups Effects on SPs of fuels :(a) pure compounds and (b) blends

Table 1: Final model hyperparameters that have been optimized

Parameter	Description
Hidden layers	1
Neurons	10
Epochs	317

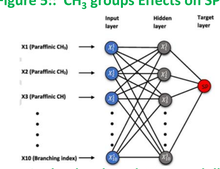


Figure 6 :The developed ANN model's finalized parameters

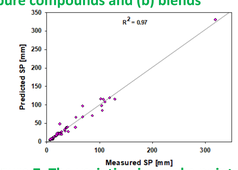


Figure 7: The variation in smoke points (SPs) between predicted and measured smoke points

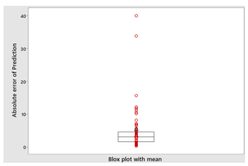


Figure 8: The difference between the measured and expected smoke point (SP) values in terms of absolute error

Summary

An artificial neural network (ANN) model was developed using the functional groups of paraffinic CH, paraffinic CH_2, paraffinic CH_3, naphthenic CH-CH_2, olefinic -CH=CH_2, aromatic C-CH, alcohol OH, and ether -O- as well as the molecular weight (MW) and branching index (BI) as the 10 features. The model was created using a dataset of 357 points, which included 236 surrogate fuel mixes and 121 pure chemicals. The model was trained using 70% and validated using 15% of the data, respectively. The model was then tested using the remaining 15 percent. One hidden layer, 10 neurons, and 317 epochs were the final parameters for the revised ANN model. Between the experimental and projected smoke spots (SPs), the correlation factor (R^2) was approximately 97%. Around 4.5 was the average absolute error. If the functional groups of the compounds are known, the created model can be used to predict the SPs of oxygenated compounds, whether they are pure or mixed. As a result, biomass fuels like ethanol and ether are likely to be mixed in with the fuels that have been screened to reduce soot.

Ongoing Work

- Using the Smoke Point Lamp to measure the smoke points (SPs) of diesel-oxygenated fuel (ASTM D1322).
- Developing an artificial neural network (ANN) model to forecast diesel-ether mixtures' propensity to soot.