Estimation of biodiesel properties from chemical composition – An artificial neural network (ANN) approach

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Abstract: Biodiesel, produced from renewable feedstock represents a more sustainable source of energy and will therefore play a significant role in providing the energy requirements for transportation in the near future. Chemically, all biodiesels are fatty acid methyl esters (FAME), produced from raw vegetable oil and animal fat. However, clear differences in chemical structure are apparent from one feedstock to the next in terms of chain length, degree of unsaturation, number of double bonds and double bond configuration—which all determine the fuel properties of biodiesel. In this study, prediction models were developed to estimate kinematic viscosity of biodiesel using an Artificial Neural Network (ANN) modelling technique. While developing the model, 27 parameters based on chemical composition commonly found in biodiesel were used as the input variables and kinematic viscosity of biodiesel was used as output variable. Necessary data to develop and simulate the network were collected from more than 120 published peer reviewed papers. The Neural Networks Toolbox of MatLab R2012a software was used to train, validate and simulate the ANN model on a personal computer. The network architecture and learning algorithm were optimised following a trial and error method to obtain the best prediction of the kinematic viscosity. The predictive performance of the model was determined by calculating the coefficient of determination ($R^2$), root mean squared ($RMS$) and maximum average error percentage ($MAEP$) between predicted and experimental results. This study found high predictive accuracy of the ANN in predicting fuel properties of biodiesel and has demonstrated the ability of the ANN model to find a meaningful relationship between biodiesel chemical composition and fuel properties. Therefore the model developed in this study can be a useful tool to accurately predict biodiesel fuel properties instead of undertaking costly and time consuming experimental tests.

Key Words: Biodiesel, Kinematic viscosity, Artificial Neural Network (ANN), Prediction model