Simulation of Biodiesel Mixtures Formulation using Artificial Neural Networks

Artificial neural networks (ANN) have been acknowledged as successful tools in the simulation of complex systems, such as biodiesel. This work was aimed at the evaluation of Artificial Neural Networks (ANN) performance in the formulation of biodiesel blends derived from different raw materials. The relevance of this study is highlighted for two major reasons. The first refers to the biodiesel quality. In cold climates, the biodiesel may undergo crystallization, a phenomenon that is the biggest limiting factors for the biodiesel use in temperate to cold climates. Crystallization is one of the requirements for biodiesel quality control. Formulation of biodiesel blends derived from different fats and oils can improve such a crystallization properties. The second relevance reason is the actual models for crystallization properties calculation portray several limitations. In fact, the using the solid-liquid equilibrium theory, blends crystallization presents a very high deviation from the ideal behavior which imposes limitations on current phenomenological or thermodynamic models. Otherwise, models for calculation of physical properties of biodiesels developed by ANN have been identified as efficient and highly accurate.

In this study, the melting/crystallization profile of a sample can be obtained, allowing the construction of a dataset of temperatures and fractions solids of samples at different compositions. In this work the dataset consisted of a set of 18194 responses. The target of the model is the fraction of solids in the mixture, given the composition and temperature. Mixtures at different composition here were composed of 11 ethyl biodiesels of Macauba, Palmiste, Soybean, Bovine tallow, Coconut, Rapeseed, Ucuuba, Peanut, Sunflower and Pinhão-Manso oils. The MATLAB was used to implement a Multilayer Perceptron with a Levenberg-Marquardt training algorithm. The ANN was training with 75% of the database and validation with the 25% of the database. The performance and accuracy was measured with the correlation coefficient. The best architecture tested was 11-10-1, that shows the results with a $R^2 > 0.99$. The proposed RNA had an excellent performance in predicting the solids content of biodiesel blends, allowing its use with confidence in the formulation of blends with low solids content that can be used at low temperatures.