Modeling the Surface Tension of Pure Liquids Using an Artificial Neural Network

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In this work, a modeling approach based on the use of an artificial neural network (ANN) was developed to estimate the surface tension value of pure liquids within a wide temperature range from the triple point up to the critical point corresponding to organic compounds of the non-polar and polar type. All ANN topologies considered in this work were generated by means of a commercial simulator called QNET 2000 which allows the construction of multi-layer, back-propagation ANNs using supervised training and the choice of various node's transfer functions. After extensively considering the combined effect of various input descriptors, ANN designs and transfer functions, finally, a three-layer feed-forward neural-network arrangement was devised and trained using 839 surface tensions of various pure liquids at different temperatures (taken from experimental sources and reference data). As a matter of fact, 25 instances out of 839 were used as test cases to check possible overtraining and integrity of the resulting ANN. The final ANN design was therefore validated during the correlation and/or the prediction of experimental surface tensions of 80 organic compounds (44 non-polar and 36 polar) at different temperatures with overall values of the root mean square error (RMS) of 0.0073 dynes/cm for the training data and 0.0116 dynes/cm for the test data based on a total of 839 experimental points. The agreement between predicted and observed surface tension data was also highly acceptable thus demonstrating the predictive abilities of the present ANN. Finally, as compared with other deterministic models available from the literature, the ANN-based model developed here proved to give somewhat improved surface tension predictions for some selected compounds. This is a remarkable result since all deterministic models considered here are predictive (except the Yaws correlation) and some of them are too cumbersome to use in comparison to the present approach.