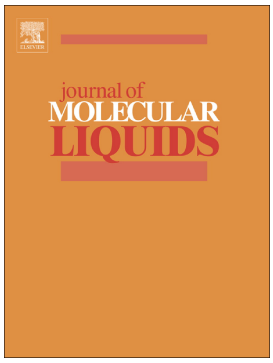

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Development of Robust Generalized Models for Estimating Normal Boiling Point of Pure Chemical Compounds

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Abstract - In this communication, four different new generalized methods are developed to predict normal boiling point of pure chemical compounds by using multilayer perceptron (MLP) and radial basis function (RBF) neural networks, least square support vector machine (LSSVM) and group method of data handling (GMDH). In order to develop the models, experimental data of 563 pure compounds are gathered from literature sources. The collected data includes experimental data points from 13 different groups including: paraffins; cycloparaffins; monooleffins and dioleffins; cyclooleffins and actylens; benzene derivatives; condensed ring aromatics and derivatives; acids, alcohols, and phenols and aldehydes; amines and nitrogen containing compounds; esters; ethers, ketones; halogenated hydrocarbons; and sulfur containing hydrocarbons. The prediction results using the proposed models are compared to three of the previously developed methods in estimating normal boiling point using statistical and graphical error analyses. Comparisons show that all of the proposed models are more reliable and accurate than the available methods. Average absolute percent relative error of the proposed MLP, RBF, LSSVM and GMDH are only 3.41%, 2.65%, and 3.11% and 3.78%, respectively. The developed method based on RBF is selected as the most accurate predictive model, while the GMDH model has the advantage of predicting normal boiling point through a simple mathematical correlation without any need to computers. To find out the outliers and applicability domain of the proposed models and prove that our models are statistically valid, Leverage approach is used. The results indicate that only small percent of the experimental dataset are located out of the applicability domain of the developed models.

Keywords - Normal boiling point; multilayer perceptron; radial basis function; least square support vector machine; group method of data handling.

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