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# Generalized Models for Predicting the Critical Properties of Pure Chemical Compounds

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**Abstract** - Critical properties of chemical compounds are of great importance as they are necessary for estimating large variety of thermodynamic and physical properties by equations of state or theorem of corresponding states. These properties are important in optimum design, operation and control of every piece of equipment in petroleum and chemical industries. In this communication, four intelligent models including radial basis function (RBF) and multilayer perceptron (MLP) neural networks, least square support vector machine (LSSVM) and hybrid group method of data handling type neural network (GMDH-PNN) are used to develop predictive models for estimation of the critical properties of pure compounds including critical temperature, critical pressure, and critical volume. A comprehensive data set of 563 pure compounds from 13 different chemical groups has been used to develop rigorous and reliable predictive models. Three easily measurable properties (normal boiling point, molecular weight, and specific gravity) were chosen as input parameters of the proposed models. The results illustrate that all of the developed models have high accuracy in predicting the critical properties, while the developed RBF models are the most accurate ones and GMDH-PNN models are the simplest models in the form of simple mathematical correlations. Comparison of the proposed models in this study with the previously developed models shows the high superiority of the proposed models. The influence degree of each input parameter on the models' outputs was investigated quantitatively using the relevancy factor. Finally, the Leverage approach was used to find out applicability domain and probable outliers of the developed models. It was found that only small percent of the data are located out of the applicability domain of the developed models.

**Keywords** - Critical properties; radial basis function; multilayer perceptron; least square support vector machine; group method of data handling

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