عنوان مقاله:

A new GA-ANN model for density prediction of organic compounds

محل انتشار:

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خلاصه مقاله:

The thermodynamic studies are important for efficient design of chemical processes, and todevelop correlation and prediction methods applicable over wide temperature and pressureranges. Among others, volumetric properties such as density and its derivatives are of greatinterest not only for industrial applications but also for fundamental aspects [1]. One of the mostwidely used methods to estimate various physical and chemical properties is quantitativestructure-property relationship (QSPR) methodology. In QSPR methodology, the property underconsideration is correlated using some chemical structure-based parameters [2]. Since, therelationship between the structural- based parameters and thermodynamic properties is highlynonlinear, an artificial neural network (ANN) can be a suitable alternative to model theunderlying thermodynamic properties [3].In this work, genetic algorithm (GA) and artificial neural network (ANN) were successfullydeveloped for density prediction of organic compounds. A large number of molecular descriptorswere calculated with Dragon software and a subset of calculated descriptors was selected from22 classes of Dragon descriptors by employing genetic algorithm analysis with partial leastsquare (GA-PLS) method from a pool of theoretically derived descriptors. Only 9 descriptorswere obtained by genetic algorithm (GA) as the most feasible descriptors, and then they wereused as inputs for neural network. Data points of density at different temperatures and pressureshave been used to train validate and test the model. The predictive model was built using theBayesian Regularized artificial neural network and its architecture and parameters wereoptimized using training set and validation set. Then, the prediction ability of the model wasevaluated using the test data sets. The mean square error (MSE) and were 43.1302, 0.9976forthe test data set. The obtained results showed the excellent prediction ability of .the proposedmodel in the prediction of density for different organic compounds

کلمات کلیدی:

genetic algorithm (GA), Organic Compounds, Artificial Neural Network (ANN), Density