عنوان مقاله:

Prediction of Polycyclic Aromatic Hydrocarbons Solubility in Supercritical Carbon Dioxide Using Artificial Neural Network (ANN) Model

محل انتشار:

دومین کنفرانس بین المللی فناوری های نوین در علوم (سال: 1397)

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خلاصه مقاله:

The polycyclic aromatic hydrocarbons solubility in supercritical carbon dioxide is crucial in a wide range of applications such as extraction from polluted soils and catalytic hydrogenation in petrochemical industry [1]. In this paper an ANN model with 7 neurons in the hidden layer and 4 input properties (temperature, pressure, critical pressure, density and acentric factor) is proposed for the prediction of polycyclic aromatic hydrocarbons solubility in supercritical carbon dioxide. A total amount of 610 data for 11 polycyclic aromatic compounds were used for training and testing the network model. 75% of the whole data (458 data) allocated for training part and the rest (152 data) used as test data. Since the values of the solubility are near to zero, logarithmic data for solubility were used for analyses. Average absolute deviation (AARD) is selected as the criteria for the accuracy of the model and is calculated as follows: ???? (%)= 100?·Σ|??????–?????|???????=1 (1) Results show that the ANN model has an average absolute deviation (AARD) of 1.06%, 1.08%, and 1.01% for all, train and test data respectively. As can be seen in figure 1, the predicted values of proposed model are close to experimental data, Therefore ANN can be an appropriate tool for predicting polycyclic aromatic hydrocarbons solubility in supercritical carbon dioxide.

کلمات کلیدی:

ANN; polycyclic aromatic; hydrocarbons; solubility; supercritical carbon dioxide