Development of hybrid machine learning model for simulation of chemical reactors in water treatment applications: Absorption in amino acid

ABSTRACT

Separation and capture of CO2 from gas mixtures is of great importance from environmental point of view which can be effectively achieved using amino acids as new class of chemical absorbents. However, screening the proper absorbent with desired separation properties using experimental measurements is tedious and costly. The predictive computational techniques can be employed to overcome this problem. In this study, for estimating and analyzing CO2 solubility in chemical solvents based on amino acid salt solutions, we created two regression models from different classes of machine learning methods. The main aim is to analyze the effect of physico-chemical parameters on the CO2 dissolution in solvent which can be carried out in chemical reactors for separation/conversion of CO2 for environmental applications. A number of CO2 solubility data are collected from resources and used for training and validation of machine learning computations. Several inputs were considered for the developed machine learning models. Inputs in this regression task are T (temperature), weight% (overall mass percentage of solvent), PCO2 (partial pressure of CO2 in the gas), MW-am (molecular weight of amino acid salt), MPC (melting point of amino acid salt), MWC (molecular mass of cation). In this task, we must predict alpha (CO2 loading in the amino acid solution) as the only output of the developed models. The models studied in this research are the Gaussian process and the decision tree boosted with Gradient boosting. With the R 2 criterion, the scores of the two Gradient boosting and Gaussian process models were obtained 0.985 and 0.993, respectively. As the third efficiency metric of the models, the Gradient boosting and regression of the Gaussian process with theRMSE criterion is the error rates of 1.10E−01 and 1.44E−01. The models developed in this work indicated to be reliable and robust enough for screening the solvents for a particular application and to save time and cost of experimental measurements.