Optimization and design of machine learning computational technique for prediction of physical separation process

ABSTRACT

Machine learning (ML) methods were developed and optimized for description and understanding a physical separation process. Indeed, this work indicates application of machine learning technique for a real physical system and optimization of process parameters to achieve the target. A bunch of datasets were extracted from resources for physical adsorption process in removal of impurities from water as a case study to test the developed machine learning model. The case study process is adsorption process which has extensive application in science and engineering. The machine learning (ML) method was developed, and the parameters were optimized in order to get the best simulation's performance for adsorption process. The data are used to correlate the adsorption capacity of the material to the adsorption parameters including dosage and solution pH. Randomized training and validation were performed to predict the process's output, and great agreement was obtained between the predicted values and the observed values with R2 values greater than 0.9 for all cases of training and validation at the optimum conditions. Three different machine learning techniques including Random Forest (RF), Extra Tree (ET), and Gradient Boosting (GB) were employed for the adsorption data. Quantitatively, R2 scores of 0.958, 0.998, and 0.999 were obtained for RF, GB, and ET, respectively. It was indicated that GB and ET models performed almost the same and better than RF in prediction of adsorption data.