Multiple machine learning models for prediction of CO2 solubility in potassium and sodium based amino acid salt solutions

ABSTRACT

In this work, we developed artificial intelligence-based models for prediction and correlation of CO2 solubility in amino acid solutions for the purpose of CO2 capture. The models were used to correlate the process parameters to the CO2 loading in the solvent. Indeed, CO2 loading/-solubility in the solvent was considered as the sole model's output. The studied solvent in this work were potassium and sodium-based amino acid salt solutions. For the predictions, we tried three potential models, including Multi-layer Perceptron (MLP), Decision Tree (DT), and AdaBoostDT. In order to discover the ideal hyperparameters for each model, we ran the method multiple times to find out the best model. R2 scores for all three models exceeded 0.9 after optimization confirming the great prediction capabilities for all models. AdaBoost-DT indicated the highest R2 Score of 0.998. With an R2 of 0.98, Decision Tree was the second most accurate one, followed by MLP with an R2 of 0.9.