Machine learning model for design of SMB processes and its application to separate rebaudioside A and stevioside

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October 24, 2020

Abstract

Several machine learning algorithms were used to simulate the simulated moving bed (SMB) process, with the sugar separation of rebaudioside A and stevioside and enantioseparation of 1,1'-bi-2-naphthol racemate as case studies. It was found the random forest (RF) model and the deep neural network (DNN) model give satisfactory accuracy with MAEs lower than 0.19% (RF) and 0.08% (DNN). Then these two models were used to optimize the operation conditions for maximizing the feed flowrate under specific purity requirements. The RF model failed to give a set of operation conditions better than the training dataset. But the DNN model gave flowrates about 10% higher than the highest values in the training datasets, for both sugar separation and enantioseparation systems. Finally the optimized operation conditions for sugar separation were verified experimentally, with the final purities of rebaudioside A and stevioside being 99.2% and 98.8% respectively.
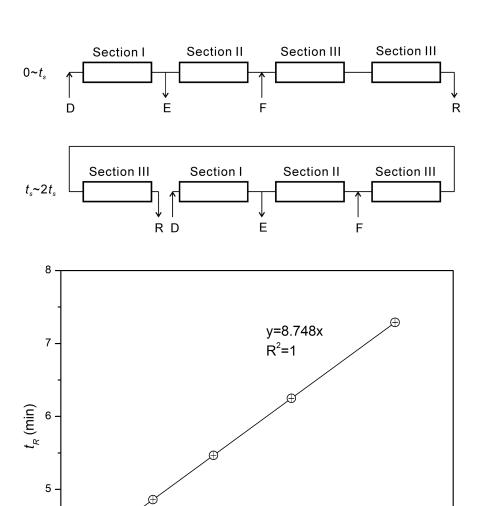
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a) Rebaudioside A   b) Stevioside

3

Input layer   hidden layers   output layer

(a) Comparision of target and predited extract purity for the sugar separation process

(b) Comparision of target and predited raffinate purity for the sugar separation process

(c) Comparison of target and predicted extract purity for the enantioseparation process

(d) Comparison of target and predicted raffinate purity for the enantioseparation process