

Prediction of chromatographic behaviors with Langmuir-artificial neural network adsorption isotherm models

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Abstract

In order to accurately predict the complex chromatographic behaviors of the components to be separated, by the combination of the Langmuir adsorption formula and the back propagation-artificial neural network (BP-ANN), Langmuir-BP-ANN adsorption model was established. Herein, based on a series of different traditional adsorption isotherms such as with or without competition, one or two kinds of adsorbed sites, monomolecular or multimolecular adsorption, and so on, the Langmuir adsorption formula was deduced, where the major adsorption parameter C_i was the function of the component concentration, expressed as matrix forms constructed by BP-ANN and obtained by solving the equilibrium dispersive (ED) chromatography model with the inverse method and genetic algorithm (GA). The Langmuir-BP-ANN model was applied to study chromatographic behaviors of m-cresol and p-cresol on MIL-53 (Al) stationary phase.

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