

# Mapping the Limitations of Breakthrough Analysis in Fixed-Bed Adsorption

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## Abstract

In a recent publication (Limitations of Breakthrough Curve Analysis in Fixed-Bed Adsorption, *Ind. Eng. Chem. Res.* 2016, 55, 4734-4748) the authors discussed the a priori prediction of the axial dispersion coefficient from available correlations versus obtaining it and also mass transfer information from experimental breakthrough data and the consequences that may arise when doing so based on using a 1-D axially dispersed plug flow model and its associated Danckwerts outlet boundary condition. These consequences mainly included determining the potential for erroneous extraction of the axial dispersion coefficient and/or the LDF mass transfer coefficient from experimental data, especially when non-plug flow conditions prevailed in the bed. Two adsorbent/adsorbate cases were considered, i.e., CO<sub>2</sub> and H<sub>2</sub>O vapor in zeolite 5A, because they both experimentally exhibited significant non-plug flow behavior, and the H<sub>2</sub>O-zeolite 5A system exhibited unusual concentration front sharpening that destroyed the expected constant pattern behavior (CPB) when modeled with the 1-D axially dispersed plug flow model.

In the current work, relationships to define the threshold values, or largest permissible values to obtain physically consistent simulation results, for the axial dispersion coefficient  $DL$  and the linear driving force coefficient  $kn$  are determined for various sorbent/sorbate systems. By keeping the values of  $DL$  and  $kn$  below these threshold values, non-physical and therefore non-predictive simulation results may be avoided in the design of gas separation processes. In order to generalize the threshold value relationships to any sorbate/sorbent system, the equilibrium capacity isotherm is approximated by the separation factor. Finally, a relationship between the threshold value and the separation factor is developed. The practical use of this relationship is the ability to determine the physical/non-physical threshold for any sorbate/sorbent pair through calculation of its separation factor.