On the Limitations of Breakthrough Curve Analysis in Fixed-Bed Adsorption

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Abstract

This work examined in detail 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 in the COMSOL Multiphysics® software 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., CO2 and H2O vapor in zeolite 5A, because they both experimentally exhibited significant non-plug flow behavior, and the H2O-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.

Overall, this work showed that it was possible to extract accurate mass transfer and dispersion information from experimental breakthrough curves using a 1-D axial dispersed plug flow model when they were measured both inside and outside the bed. To ensure the extracted information was accurate, the inside the bed breakthrough curves and their derivatives from the model were plotted to confirm whether or not the adsorbate/adsorbent system was exhibiting CPB or any concentration front sharpening near the bed exit. Even when concentration front sharpening was occurring with the H2O-zeolite 5A system, it was still possible to use the experimental inside and outside the bed breakthrough curves to extract fundamental mass transfer and dispersion information from the 1-D axial dispersed plug flow model based on the systematic methodology developed in this work.

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Figures used in the abstract

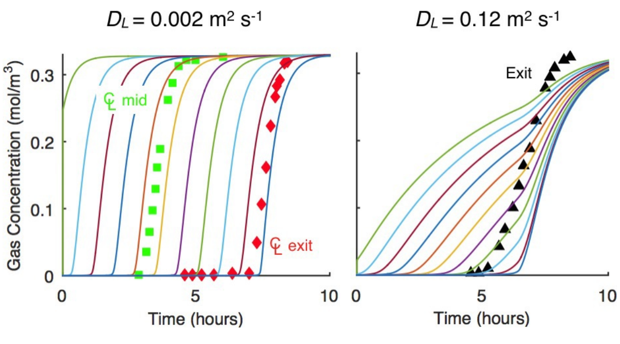

Figure 1: Breakthrough curve simulation with variations in axial dispersion coefficient compared with centerline and exit concentrations.

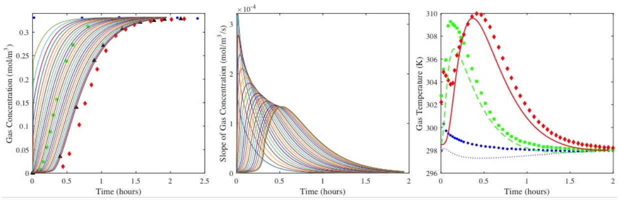

Figure 2: CO2 on zeolite 5A: Fit of the 1-D axial dispersed plug flow model to the outside bed (triangles) experimental breakthrough curve using a value of DL 7 times greater than that from the Wakao and Funazkri correlation (left) and the fitted LDF kn = 0.0023 s-1.

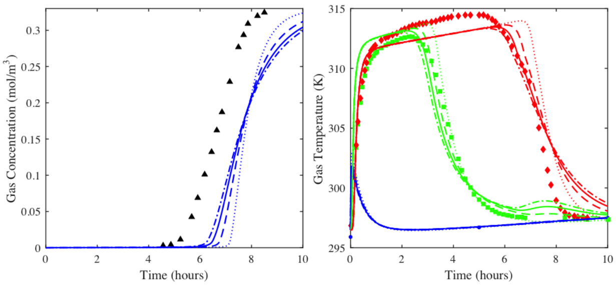

Figure 3: H2O vapor on zeolite 5A: Predictions from the 1-D axial dispersed plug flow model of the outside bed (triangles) experimental breakthrough curve when varying the value of DL. DL = 10 (dotted lines), 30 (dashed lines), 50 (solid lines) and 70 (dash-dot lines) times greater than Wakao and Funazkri correlation.

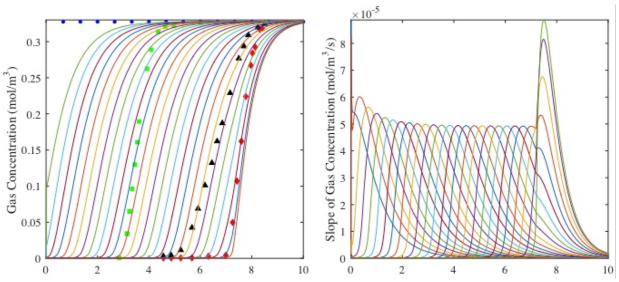

Figure 4: H2O vapor on zeolite 5A: Predictions from the model (lines) of the gas phase concentration breakthrough curves at 0, 4, 8, 12, ... 92, 96 and 100% locations in the bed.