Supporting Information:
Prediction of non-isothermal ternary gas-phase breakthrough experiments based on binary data

*Adsorption*

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1 Validation of the used heat transfer correlation

A comparison of the description of experiment B5 and B22 with the heat transfer coefficient calculated by the correlation as reported in Casas et al (2012) and with the individually fitted heat transfer coefficient.
Figure S1: Experimental (symbols) and simulated results of breakthrough experiments B5 (a) and B22 (b). Simulations carried out with the predicted heat transfer coefficient from Eq. 2 (solid lines) are compared to the simulated profiles with the individually fitted $h_L$ shown in Figure 2.
2 Binary breakthrough experiments

In this section the full set of experimental results for the binary mixtures is presented together with the simulations obtained by fitting the mass transfer coefficients. To obtain the experimental data in a digital form, interested readers are invited to contact the authors.
Figure S2: Experimental (◦) and simulated (-) results of breakthrough experiments with the binary mixture containing 10/90 CO₂/N₂ at a temperature of 25 °C. The top row shows the exit profiles of the experiments performed at various levels of pressure and flow rate, while the bottom row shows the corresponding temperature profiles.
Figure S3: Experimental (○) and simulated (-) results of breakthrough experiments with the binary mixture containing 10/90 CO$_2$/N$_2$ at a temperature of 45°C. The top row shows the exit profiles of the experiments performed at various levels of pressure and flow rate, while the bottom row shows the corresponding temperature profiles.
Figure S4: Experimental (◦) and simulated (-) results of breakthrough experiments with the binary mixture containing 50/50 CO$_2$/N$_2$ at a temperature of 25°C. The top row shows the exit profiles of the experiments performed at various levels of pressure and flow rate, while the bottom row shows the corresponding temperature profiles.
Figure S5: Experimental (◦) and simulated (-) results of breakthrough experiments with the binary mixture containing 50/50 CO$_2$/N$_2$ at a temperature of 45°C. The top row shows the exit profiles of the experiments performed at various levels of pressure and flow rate, while the bottom row shows the corresponding temperature profiles.
Figure S6: Experimental (◦) and simulated (—) results of breakthrough experiments with the binary mixture containing 80/20 \( \text{CO}_2/\text{N}_2 \) at a temperature of 25°C. The top row shows the exit profiles of the experiments performed at various levels of pressure and flow rate, while the bottom row shows the corresponding temperature profiles.
Figure S7: Experimental (◦) and simulated (-) results of breakthrough experiments with the binary mixture containing 80/20 CO₂/N₂ at a temperature of 45°C. The top row shows the exit profiles of the experiments performed at various levels of pressure and flow rate, while the bottom row shows the corresponding temperature profiles.