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Jelan Kuhn,* Juan Manuel Castillo-Sanchez, Jorge Gascon, Sofia Calero, David Dubbeldam, Thijs J. H. Vlugt, Freek Kapteijn, and Joachim Gross*: Adsorption and Diffusion of Water, Methanol, and Ethanol in All-Silica DD3R: Experiments and Simulations

Page 14290. We have recently found errors in the computation of some of the adsorption isotherms reported in our original paper.[1] In some simulations, the blocking of the inaccessible cages[2] of the DDR zeolite was not performed correctly. The adsorption of water and ethanol at high fugacities, and the water/methanol and water/ethanol mixture isotherms, are affected. This corresponds to Figures 6, 7, and 8 of the original manuscript. The computed pure component isotherms at low fugacity, self-diffusivities, permeate side compositions, thermodynamic correction factors, and average enthalpies of adsorption at zero loading are not affected. The main conclusion of the study remains unchanged; i.e., the separation performance of water/alcohol mixtures in DDR membranes is due to different diffusion coefficients of the molecules adsorbed rather than to differences in adsorption.

We have recalculated the data presented in Figures 6, 7, and 8 using a correct blocking of the inaccessible cages.[2] The saturation loading calculated at a fugacity of 1 GPa and 303 K yields saturation loadings of 10.4, 4.2, and 2.6 mol$\cdot$kg^{-1} for water, methanol, and ethanol, respectively (Figure 6), corresponding to 25, 10, and 6 molecules per 19-hedra cage, respectively. Figures 7 and 8 show methanol/water and ethanol/water mixture isotherms respectively at low total fugacity, and water feed fractions Y_w between 0.1 and 0.5. The water loading increases with the water fugacity ratio, while the alcohol loading shows only a slight decrease and the shape of the alcohol isotherm remains the same as for the single-component adsorption. The water adsorption is enhanced by the presence of alcohol, while the alcohol adsorption is practically insensitive to the presence of water, showing a small enhancement in the case of ethanol.

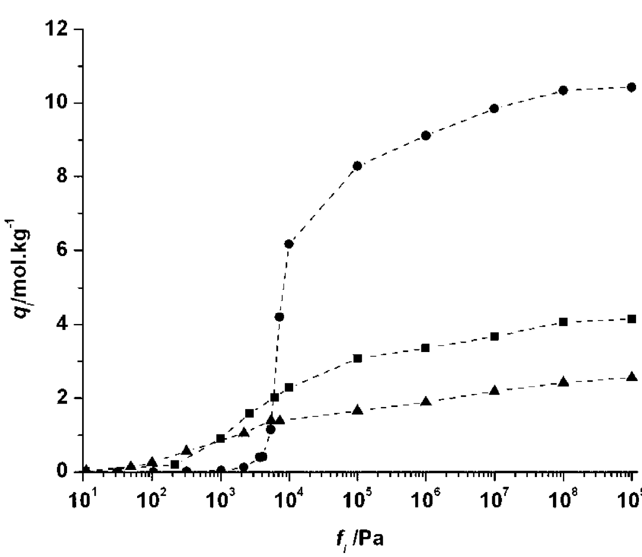

Figure 6. Water (circles), methanol (squares), and ethanol (triangles) adsorption isotherms up to 1 GPa at 303 K. The lines are a guide to the eye.

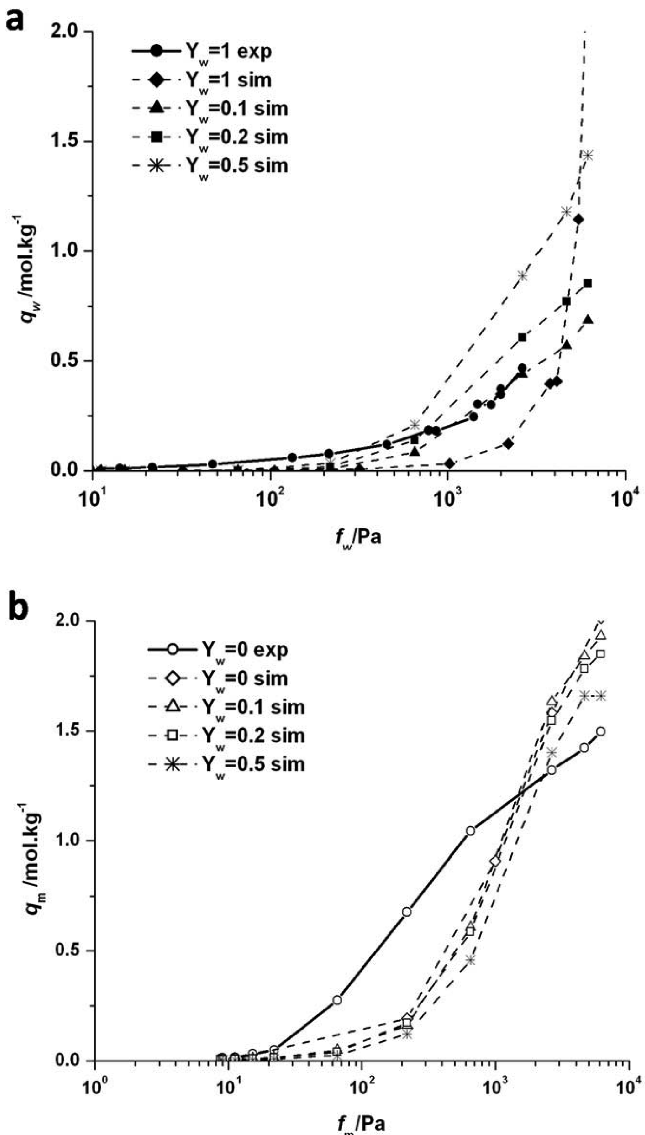

Figure 7. Experimental (exp) pure-component and calculated (sim) methanol/water adsorption isotherms at 303 K for water fugacity rations of $Y_w = 0$, 0.1, 0.2, 0.5, and 1. The loading of (a) water and (b) methanol is shown as a function of the component fugacity. The solid lines indicate the experimental pure-component isotherms. The lines are a guide to the eye.

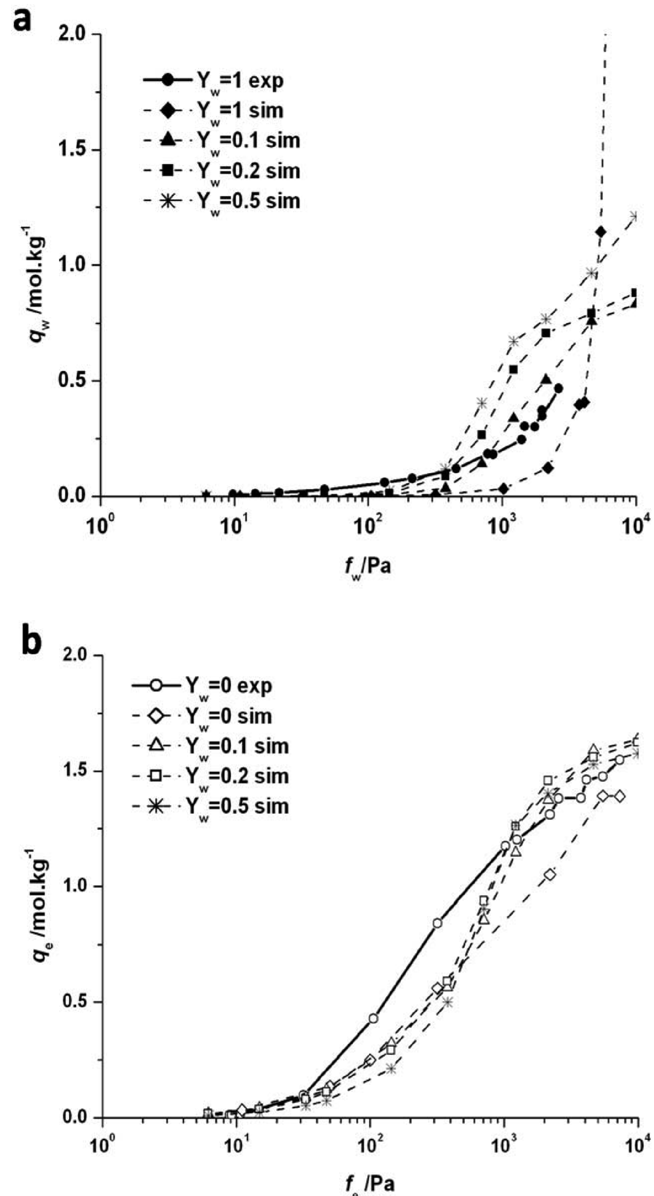

Figure 8. Experimental (exp) pure-component and calculated (sim) ethanol/water adsorption isotherms at 303 K for water fugacity ratios of $Y_w = 0$, 0.1, 0.2, 0.5, and 1. The loading of (a) water and (b) ethanol is shown as a function of the component fugacity. The solid lines indicate the experimental pure-component isotherms. The lines are a guide to the eye.

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References and Notes

(1) Kuhn, J.; Castillo-Sanchez, J. M.; Gascon, J.; Calero, S.; Dubbeldam, D.; Vlugt, T. J. H.; Kapteijn, F.; Gross, J. *J. Phys. Chem. C* **2009**, *113*, 14290.
(2) Jakobtorweihen, S.; Hansen, N.; Keil, F. J. *Mol. Phys.* **2005**, *103*, 471.

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