**Transport coefficients of *n*-butane into and through the surface of silicalite-1 from non-equilibrium molecular dynamics study**

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The aim of this work was to investigate the transport properties into and through the surface of a zeolitic material. As a model system we have chosen an important system, namely silicalite-1 in contact with *n*-butane gas.
Gradients of temperature and concentrations were created across the surface using non-equilibrium molecular dynamics algorithms developed for the purpose. A description of the surface was given using non-equilibrium thermodynamics.
A comparison between equilibrium and non-equilibrium results confirmed that the surface was in local equilibrium and could be regarded as a thermodynamic system.
For the first time, coefficients for the coupled transport of heat and mass were reported for a zeolite-gas interface.
Three independent coefficients were found for transport across the whole surface: the resistance to heat transfer, the coupling coefficient and the resistance to mass transfer. All resistances were significant, and showed that the surface acted as a barrier to transport.
A new scheme was devised to find the enthalpy of adsorption from two measurable heats of transfer for the whole surface using either the heat fluxes on the gas or the zeolite sides. The method yielded the enthalpy of adsorption as a function of the excess surface concentration and surface temperature.
A further inspection of the surface, regarded as a series of two resistances, one on the gas and one on the zeolite side was made. It showed that the gas side of the surface dominated the overall resistance to heat transfer, while the zeolite side, which was characterized by negative excess concentrations, dominated the overall resistivity to mass transfer and determined the value of the coupling coefficient.
The coefficients were found not to be sensitive to the surface structure, whether it was flat, or zig-zag textured.
The findings may help reduce adsorption data from experiments on zeolites and other porous materials.

[1] I. Inzoli, J-M.Simon, S. Kjelstrup, D. Bedeaux, J. Colloid Interface Sci. 2007, 313, 563.
[2] S. Kjelstrup, D. Bedeaux, Non-Equilibrium Thermodynamics of Heterogeneous Systems; World Scientific, 2008; Vol. 16.
[3] I. Inzoli, J-M. Simon, S. Kjelstrup and D. Bedeaux, J. Phys. Chem. B 112 (2008) 14937.
[4] I. Inzoli, S. Kjelstrup, D. Bedeaux, J-M. Simon, Microporous and Mesoporous materials, 2009,125, 112
[5] I. Inzoli, J-M. Simon, S. Kjelstrup, Langmuir 2009, 25, 1518.