Information on Diffusion Phenomena Available by Neutron Scattering

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The diffusion coefficient of molecules adsorbed in zeolites can be obtained from the broadening of energy spectra measured at different momentum transfer values. The technique is called quasi-elastic neutron scattering (QENS) because small energy transfers are involved. During the QENS experiments, one probes molecular diffusion over space scales ranging from a few Å to several nm. At short distances, jumps between adsorption sites can be observed, so that the characteristic lengths and times of the elementary steps can be determined using jump diffusion models. Such jump processes can be modelled by simulation techniques, which makes comparisons between QENS and simulations very fruitful. Over space scales of a few unit cells, Fickian diffusion is observed so that the diffusion coefficients can be derived without a model.

The technique was first used to obtain self-diffusivities of hydrocarbons, because of the large incoherent cross section of hydrogen. However, transport diffusivities of molecules which do not contain hydrogen atoms can also be derived, thanks to the high neutron flux available on recent spectrometers. One can cite for example CO_2, CF_4, N_2 and O_2. The neutron results indicate that the corrected diffusivity is rarely constant.

Another neutron technique which has been used recently to derive diffusivities in zeolites is the neutron spin-echo (NSE) technique. It has been found that NSE pushes down the lower limit of diffusion coefficients accessible by neutron methods by two orders of magnitude. Using different spectrometers, one can now cover time scales ranging from femtoseconds to microseconds.