"PFG NMR Study of Long-Range Diffusion in Beds of NaX Zeolite: Evidence for Different Apparent Tortuosity Factors in the Knudsen and Bulk Regimes" Oliver Geier, Sergey Vasenkov, Jörg Kärger J. Chem. Phys. 118 (2003) 6129

A traditional approach to the tortuosity factor in chemical engineering literature is based on the assumption that this factor reflects intrinsic geometrical properties of the porous structure and thus does not depend on the diffusion regime (Knudsen or bulk). However, the results of a number of recent dynamic Monte Carlo simulations of gas diffusion in porous media have shown that the tortuosity factor in the Knudsen regime can be several times larger than that in the bulk regime for the same porous system (V.N. Burganos, J. Chem. Phys. 109 (1998) 6772, G.L. Vignoles, J. Phys. IV 5 (1995) 159, M.M. Tomadakis and S.V. Sotirchos, AIChE J. 39 (1993) 397). In the present work we report for the first time the experimental data, which supports these simulation results.

Self-diffusion of ethane in beds of zeolite NaX was studied using Pulsed Field Gradient (PFG) NMR. The ethane diffusivities were measured for displacements, which are orders of magnitude larger than the size of individual crystals. These diffusivities were compared with those, calculated using simple gas kinetic theory. The results of the comparison indicate that for the same bed of NaX crystals the apparent tortuosity factor in the Knudsen regime (i.e. when molecule-solid collisions dominate) is significantly larger than that in the bulk regime (i.e. when molecule-molecule collisions dominate). This finding may be rationalized by noting that the momentum exchange between the gas molecules and the pore walls proceeds much more effectively in the Knudsen than in the bulk regime. Therefore the diffusion resistance imposed by the walls may also be larger in the Knudsen regime. (© Vasenkov)