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Diffusion in hierarchical silica monoliths: impact of pore size and probe molecule

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The silica monoliths were prepared by a combination of sol-gel synthesis, pore templating, and a process of phase separation. The as-prepared monoliths are characterized by meso- and macroporosity. The pore size significantly differs for each sample depending on the preparation conditions. The transport properties of the monoliths were investigated using benzene, isopropanol, hexane, and methane as probing molecules. The effective diffusion coefficients in the monoliths were estimated based on the second Fick’s law of diffusion. The obtained diffusivities are quite similar for different samples, demonstrating that the diffusion occurs mainly in the macropores of the monolith. The values of the diffusion coefficients were found to fall outside the Knudsen prediction. In addition, it was investigated that the benzene and hexane transport in the monolith sample with a bimodal mesopores distribution does not follow the Fick’s diffusion law. To describe the mass transfer of the benzene and hexane in this sample the time-fractional diffusion equation was utilized on a phenomenological basis. Several scenarios concerning the role of the relatively small mesopores in the hydrocarbons diffusion are discussed.

Metryczka

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