

Abstract Submitted
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The reversibility of the adsorption of methane-methyl mercaptan mixtures in nanoporous carbon¹ CARLOS WEXLER, MONIKA GOLEBIEWSKA, University of Missouri, LUCYNA FIRLEJ, Universite Montpellier 2, BOGDAN KUCHTA, Universite Aix-Marseille 1, MICHAEL ROTH, University of Northern Iowa — The results of extensive molecular dynamics simulations and theoretical considerations of the adsorption of methane-methyl mercaptan mixtures in slit-shaped carbon nanopores are presented. We observe significant mobility of both methane and mercaptan molecules within the pore volume, between pores, and between adsorbed and gas phases for a wide range of temperatures and pressures. Although mercaptans adsorb preferentially relative to methane, the process remains reversible, provided non-oxidizing conditions are maintained. A mercaptan/methane ratio of the order of 200 ppm in the adsorbed phase is sufficient for the gas phase to have a mercaptan concentration above the human threshold for detection. The reversibility of the adsorption process and low concentration of mercaptans makes it unlikely that these would be harmful for adsorbed natural gas storage systems. See also: doi:10.1016/j.carbon.2011.08.039.

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