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Diffusion of Small Penetrants in Polybutadienes[1] AHMED E. ISMAIL, GARY S. GREST, FLINT PIERCE, MATHEW C. CELINA, Sandia National Laboratories — Polybutadiene is a high-volume synthetic rubber with a low glass transition temperature that can be made in a wide range of forms from pure cis to pure trans conformations. In spite of its industrial importance, there is significant variance in the observed diffusivity of small penetrants through polybutadiene for both experiment and simulation. We use explicit-atom molecular dynamics simulations to model the diffusivity of the penetrants water, oxygen, and methanol in three polybutadiene systems, all *cis*-1,4, all *trans*-1,4 and a microstructure of 40% *cis*-1,4, 50% *trans*-1,4, and 10% vinyl monomeric units. In addition to varying the monomeric composition, we also study the effects of varying the chain length of the polybutadiene molecules, temperature and penetrant concentration. The trajectories of individual molecules are analyzed to determine if the "caging" and "hopping" phenomena observed by Müller-Plathe for methane in polyethylene occurs.

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