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Discontinuous molecular dynamics study of the diffusion of fluids in dynamic random media KAMAKSHI JAGANNATHAN, Graduate student, University of Wisconsin, ARUN YETHIRAJ, Professor, University of Wisconsin —
The static and dynamic properties of dimeric hard sphere fluids in random media are studied using discontinuous molecular dynamics. The media is composed of a random collection of hard spheres that are dynamic in the sense that they are connected by a string to their respective initial positions, and can move in the spherical volume defined by the length of the string, l. The fluid diffusion coefficient is calculated as a function of l for different volume fractions of the fluid and media. In the $l \to 0$ and $l \to \infty$ limits, the system reproduces the limits of a fluid in a static media and in a hard sphere liquid, respectively. Much of the phenomenology of glass forming materials is reproduced by this model. For example, this model mimics experimental studies for impurity diffusion in glass forming materials. The diffusion behavior changes from a power law behavior (in l) above a critical l to an Arrhenius behavior below this critical l.

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