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Upscale rarefied volatile diffusion in porous media: a probability-based pore network modeling approach

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In certain regions of airless bodies, such as the Moon and cometary nuclei, volatile components like water, carbon dioxide, and methanol can persist and migrate within the regolith due to extremely low temperatures[1-5]. Studying the diffusion behavior of volatiles in porous media is crucial for the exploration and exploitation of these extraterrestrial resources.

Under such extremely high vacuum conditions[6], gas molecules undergo Knudsen diffusion, where the average free path is more than 10 orders of magnitude larger than the size of regolith particles[7] (Knudsen number Kn > 1010). At this almost infinitely large Knudsen number, gas molecules rarely collide with each other, and the diffusion trajectories resemble chords (free paths) between solid surfaces, determined solely by porous structure. Additionally, the number of molecules within a single pore is too small to satisfy statistical continuity. Previous studies on Knudsen diffusion have been limited to either simple tube-like structures[8-11] or Monte Carlo simulation[12, 13] that only provide chord length distributions and effective diffusion coefficients. A direct model linking pore structure to dynamic diffusion behavior is still lacking.

We first conduct numerical experiments by employing test particle Monte Carlo (TPMC) simulations, to obtain molecular trajectories and the diffusion coefficients in complex porous media. We find that pore-bodies and pore-throat behaves very differently. Pore-bodies exhibit isotropy (the exit direction of molecules in pores is uniformly distributed) and satisfy the Markov property (the exit probability of molecules in pores is independent of their residence time), while pore-throats are anisotropic and do not satisfy Markov property.

Based on this duality of local diffusive property and the rarefied feature, we develop a probability-based pore network modeling (pb-PNM) approach to upscale Knudsen diffusion from pore-scale to representative elementary volume (REV) scale. The model uses the probability of a molecule residing in a specific structure (i.e., pore or throat) at a given time to represent the spatial distribution and transfer probability of a molecule between different structures to represent the change in the spatial distribution within a specific time period. The relative error between the predicted diffusion coefficient and the numerical experimental results is less than 20% in most cases.

This pb-PNM method leverages the characteristics of gas molecular movement in pores and throats, obtained from TPMC simulations, to scale up to larger core scales. As a result, this method can be used to analyze the effects of adsorption and heterogeneity on the diffusion of rarefied volatiles, and to simulate the unsteady diffusion process with significantly fewer computational resources compared to TPMC simulations.

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