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Volatile Transport in Porous Lunar Regolith: Diffusion at Infinite Knudsen Number

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The lunar surface is covered with a layer of lunar regolith. Observational evidence[1-3] suggests that it may contain volatile substances such as water, methane, and helium-3 that could be utilized. Studying the diffusion behavior of volatiles in lunar regolith is of great significance for the exploration and exploitation of these extraterrestrial resources.

Volatile in lunar regolith layer exist under extremely high vacuum conditions ($\sim 10^{-9}$ Pa)[4]. Under such extreme conditions, gas molecules undergo Knudsen diffusion, where the average free path is more than 10 orders of magnitude larger than the size of lunar regolith particles (Knudsen number $Kn > 10^{10}$). At this extreme (almost infinitely large) Knudsen number condition, gas molecules in porous lunar regolith rarely collide with each other, and the diffusion trajectories resemble chords (free paths) between solid surfaces which are determined solely by porous structure. Previous studies have measured tortuosity[5] or free path length distribution[6] to modify the diffusion coefficient, but the correlation between pore structure and the diffusion coefficient is still largely unexplored.

In this study, we investigate the influence of pore structure on the diffusion of rarefied gases in porous media at infinitely large Knudsen number, based on a Monte Carlo program. Numerical experiments confirm that the linear relationship between the mean square displacement and time predicted by the Einstein equation still holds. However, the statistics of free path lengths shows clear bimodal-distribution even in homogeneous media, which is different from the unimodal-distribution as shown in porous media Fickian diffusion or in straight tube Knudsen diffusion. By statistically analyzing the molecular trajectories within the porous medium, we show that the bimodal distribution corresponds to the sizes of pore and the throat.

According to the pore-throat bimodal distribution of free path length, we establish a bimodal random walk model to derive the diffusion coefficient from the pore and throat parameters. This analytical prediction successfully matches the numerical experiments with various structures. We further investigate the impact of adsorption and heterogeneity on the volatile transport in porous media at infinitely-high Knudsen number.

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