Chemosphere
Volume 349, February 2024, 140966

The effect of the initial temperature, pressure, and shape of carbon nanopores on the separation process of SiO_2 molecules from water vapor by molecular dynamics simulation

Bing Mei [a], Dheyaa J. Jasim [b], As'ad Alizadeh [c], Maboud Hekmatifar [d], Navid Nasajpour-Esfahani [e], Soheil Salahshour [f g h], Roozbeh Sabetvand [i], D. Toghraie [d]

https://doi.org/10.1016/j.chemosphere.2023.140966

Abstract

Today, with the advancement of science in nanotechnology, it is possible to remove dust nanostructures from the air breathed by humans or other fluids. In the present study, the separation of SiO_2 molecules from H_2O vapor is studied using molecular dynamics (MD) simulation. This research studied the effect of initial temperature, nanopore geometry, and initial pressure on the separation of SiO_2 molecules. The obtained results show that by increasing the temperature to 500K, the maximum velocity (Max-Vel) of the samples reached 2.47Å/fs. Regarding the increasing velocity of particles, more particles pass via the nanopores. Moreover, the shape of the nanopore could affect the number of passing particles. The results show that in the samples with a cylindrical nanopore, 20 and 40% of SiO_2 molecules, and with the sphere cavity, about 32 and 38% of SiO_2 particles passed in the simulated structure. So, it can be concluded that the performance of carbon nanosheets with a cylindrical pore and 450K was more optimal. Also, the results show that an increase in initial pressure leads to a decrease in the passage of SiO_2 particles. The results reveal that about 14 and 54% of Silica particles passed via the carbon membrane with increasing pressure. Therefore, for use in industry, in terms of separating dust particles, in addition to applying an EF, temperature, nanopore geometry, and initial pressure should be controlled.