

## **Atomistic Study of Fluid Transport in Hierarchical Porous Materials**

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Atomistic non-equilibrium molecular dynamics simulations were employed to quantify methane transport in hierarchical porous networks. Model amorphous silica materials were used as solid substrates, which allows us to construct pore networks with well-defined properties. The results show that the methane diffusivity and permeability through the pores strongly depend on the frameworks. Analysis of the vector fields for methane within the pores reveals the existence of local back-flow near the solid substrates, which disturbs methane transport. Varying the pore cross-sectional areas leads to changes in the entropy potential along the flow direction, which influences the molecular path length. The results show a linear relationship between methane transport (i.e., permeability) and a pore characteristic parameter that takes into consideration porosity, constriction factor, and tortuosity. This relation holds for hierarchical porous materials containing both micropores and mesopores. Diffusivity and permeability of methane through porous media are found to scale as a power function of porosity and constriction factor. These are measurable descriptors, suggesting that transport properties could be predicted for engineering and natural materials once characterisation data are available. For example, we show here that a power law can describe results obtained for Fontainebleau sandstone. The good agreement achieved suggests that using the approach presented here not only enables the quantification of molecular effects influencing fluid transport, but also allows the reliable prediction of diffusivity and permeability of fluids through sedimentary rocks using as sole input macroscopic pore structure information.