ICCES, 2024, vol.32, no.1
DOI: 10.32604/icces.2024.011068

PROCEEDINGS

A Generalized Knudsen Theory for Gas Through Nanocapillaries Transport

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ABSTRACT

Gas permeation through nanopores is a long-standing research interest because of its importance in fundamental science and many technologies. The free molecular flow is conventionally described by Knudsen theory, under the diffuse reflection assumption. Recent experiments reported ballistic molecular transport of gases, which urges for the development of theoretical tools to address the predominant specular reflections on atomically smooth surfaces. Here we develop a generalized Knudsen theory, which is applicable to various boundary conditions covering from the extreme specular reflection to the complete diffuse reflection [1]. Our model overcomes the limitation of Smoluchowski model, which predicts the gas flow rate diverging to infinity for specular reflection. It emphasizes that the specular reflection can reduce the dissipation flow rate. Our model is validated using molecular dynamics simulations in various scenarios. The proposed model provides insights into the gas transport under confinement and extends Knudsen theory to free molecular flow with specular reflections.

KEYWORDS

Free molecular flow; Knudsen theory; specular reflections; nanocapillaries

Funding Statement: The authors received no specific funding for this study.

Conflicts of Interest: The authors declare that they have no conflicts of interest to report regarding the present study.

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