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POROSITY EFFECT ON HEAT TRANSFER IN A NANOCHANNEL: MOLECULAR DYNAMICS SIMULATION

Abstract

This paper studies the effect of porosity on the heat transfer across a nanochannel. The investigation aims to highlight heat transfer in solid-liquid interface in a nanofluidic pore. The computational domain consists of two parallel walls with dimensionless temperature 1.3 at the top wall and 1.2 at the bottom wall thermostated with tempereture rescaling method. The system is performed with micro-canonical ensemble with simulation time of 40,000,000 and equilibration run of 4,000,000. The atoms of the walls are positioned by fcc lattice with orientation x(0 -1 1); y(1 1 1); z(-2 1 1) with spring constant k=(100-1600)$\varepsilon\sigma$-2. The initial results recorded a temperature jump at the walls of the channel. A linear temperature profile is observed across the channel for various porosity. This study will aid in the understanding of heat transfer and fluid flow in boundaries and intefaces.