Study of fluid flow in grooved micro and nano-channels via dissipative particle dynamic: a tool for desalination membrane design

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ABSTRACT

A number of recent studies strongly suggest that nanostructured materials, such as carbon nanotubes, nanoporous graphene, and zeolites, can form the basis for the fabrication of next generation membranes for reverse osmosis desalination. In the present work, we investigate the influence of the wall roughness and external driving force on the flow pattern and energy losses in nano and microchannel flow through the estimation of the effective velocity slip at solid walls and other macroscopic quantities such as density, velocity, and pressure. The investigation is based on the dissipative particle dynamics simulation method and the flow studies concern flows between parallel plates with the protrusions located at the upper wall. Roughness is modeled by periodically spaced rectangular protruding elements. When compared to the smooth channel case, lower flow velocities are observed in the central part of the channel for all cases studied. This reduction of velocities becomes more pronounced as the protrusion height increases. For the microchannel, density, pressure, and temperature remain almost constant in the central part of the channel and their pattern near and inside the cavities depends on the protrusion shape. The results show that the slip velocity, both for the nano and microchannel flow, is reduced as the protrusion length is reduced and the protrusion height is increased for both the upper rough and the lower flat wall. As far as the external driving force is concerned, it seems that the slip velocity increases as the external driving force increases for constant protrusion size. The study of these parameters is of particular importance for the design of filters and membranes based on nanomaterials employed in the desalination process as well as contaminant removal from water.

Keywords: Grooved microchannels; Nanochannels; Slip velocity; Dissipative particle dynamics; Protrusion size effect; Desalination

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