عنوان مقاله:

Effects of different atomistic water models on the velocity profile and density number of Poiseuille flow in a nano-channel: Molecular Dynamic Simulation

محل انتشار:

مجله چالش های نانو و مقیاس خرد در علوم و فناوری, دوره 5, شماره 1 (سال: 1396)

تعداد صفحات اصل مقاله: 10

نویسندگان:

H. Nowruzi - *Department of Maritime Engineering, Amirkabir University of Technology (Tehran Polytechnic), Hafez Ave, No ۴۲۴, P.O. Box ۱۵۸۷۵-۴۴۱۳, Tehran, I. R. Iran*

H. Ghassemi - *Department of Maritime Engineering, Amirkabir University of Technology (Tehran Polytechnic), Hafez Ave, No ۴۲۴, P.O. Box ۱۵۸۷۵-۴۴۱۳, Tehran, I. R. Iran*

خلاصه مقاله:

In the current study, five different atomistic water models (AWMs) are implemented, In order to investigate the impact of AWMs treatment on the water velocity profile and density number. For this purpose, Molecular dynamics simulation (MDS) of Poiseuille flow in a nano-channel is conducted. Considered AWMs are SPC/E, TIP۳P, TIP۴P, TIP۴PFQ and TIP۵P. To assessment of the ability of each model in prediction of velocity profile, it is compared with analytic velocity profile. Furthermore, MDS results of density number are evaluated by real non-dimensional value for density number of water (Rho*). Based on computational results,predicted velocity profile from MDS is in appropriate accordance to analytic solution based on the Navier–Stokes equations. In addition, SPC/E and TIP۴P models prepare the best prediction of the velocity profile, and are recommended where the averaged magnitude of velocity across the nano-channel is essential. Furthermore, a jump in velocity of TIP۵P and TIP۴P models is revealed in the vicinity of the nano-channel walls. However, approximately similar quantity is detected in the flow velocity of all different AWMs near the nano-channel walls. Finally, numerical results related to density number show, the TIP۵P water model has higher compliance with the intended Rho*, and thus this model is suggested, where density number plays an important role in our MDS.

کلمات کلیدی:

Molecular dynamics simulation, Atomistic water models, Analytic solution, Velocity profile, Density number, Lennard-Jones