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Non-equilibrium Molecular Dynamics Simulations of Channel Flows. F. SOFOS, T. KARAKASIDIS, A. LIAKOPOULOS, Dept. Civil Engineering, University of Thessaly, Volos, Greece — We present non-equilibrium molecular dynamics simulations of liquid argon flow through nano-channels formed by two infinite krypton plates. Density, velocity and temperature distributions across the channel are studied for channels widths in the range 2.65σ-18.58σ (σ is the argon atom diameter). For small channels (2.65σ-7.9σ) the fluid is ordered in layers and this ordering persists close to the walls even for wider channels. Velocity profiles in small channels deviate from the parabolic behavior predicted by continuum theory. The no-slip condition breaks down in small channels for all external forces and system temperatures studied while for large channels it is always satisfied. For channels of intermediate width the validity of the no-slip condition depends on the system temperature and the magnitude of the driving force. Temperature distribution remains uniform across the channel for values of the driving force below a threshold value which depends on channel width. We calculated also the diffusion coefficient, D, along the flow (x-direction) and across the channel (z-direction). The ratio Dz/Dx increases as the channel width increases with diffusion being higher in layers close to the center of the flow. Acknowledgment: The authors acknowledge financial support of the Hellenic Secretariat for Research & Technology under grant pened-03-uth-3337.

T. Karakasidis
Dept. Civil Engineering, University of Thessaly, Volos, Greece

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