

Simulation of a mixed water/ion Poiseuille flow system

List of symbols

C : energy conversion constant

dt : simulation time step

q_i : charge of atom i

ϵ : dielectric constant

E ; External electric field

F_{ext} ; magnitude of external driving force in the x -direction

F_e ; force due to electric field in the z -direction

h ; channel height

K : spring constant

m ; atomic mass

N ; number of particles

r_c : cut-off radius for the LJ potential

r_i ; position of atom i

r_{eq} ; initial lattice position

r_{ij} ; distance vector between i^{th} and j^{th} atom

T ; temperature

t ; time

$u(r_{ij})$: LJ potential of atom i with atom j

Greek symbols

ε ; energy parameter in the LJ potential

ρ ; fluid density

σ ; length parameter in the LJ potential