Contribution ID: **73** Type: **Poster (+) Presentation**

Effects of nanopore geometry on confined water flow: a view of lattice Boltzmann simulation

Thursday, 3 June 2021 20:00 (1 hour)

Water flow in nanoscale channel is known to be affected by the strong water-wall interactions which induces that the flow significantly deviates from the conventional continuum flow. Vast experimental observation and simulation results in recent literature shows higher/lower-than-expected flow capacity in nanopores. Currently, most research are limited on the simple geometry with circular cross section. However, the flow dynamics of water in noncircular pores deviates from the Hagen–Poiseuille flow equation used in circular pores with various contact angles and dimensions significantly. In this work, molecular interactions between water and the solid inner wall are incorporated into Lattice Boltzmann method formulations to simulate the flow dynamics in nanopore with different cross-sectional shapes and wettability. When cross-sectional area injection pressure is identical, the circular nanopore has the strongest flow capacity. For circular cross-sectional shape, the constant density lines are also circular and concentric. For angular cross-sectional shape, the constant density lines become inconsistent with cross-sectional shape, the density varies greatly at the corner. The effects of geometry and density distribution of different contact angles have been analyzed in details. An empirical formula has been established which is of great use value in engineering field.

Time Block Preference

Time Block B (14:00-17:00 CET)

References

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