Abstract Submitted
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Non-isothermal 3D SDPD Simulations[1] JUN YANG, RAFFAELE POTAMI, NIKOLAOS GATSONIS, Worcester Polytechnic Institute — The study of fluids at micro and nanoscale requires new modeling and computational approaches. Smooth Particle Dissipative Dynamics (SDPD) is a mesh-free method that provides a bridge between the continuum equations of hydrodynamics embedded in the Smooth Particle Hydrodynamics approach and the molecular nature embedded in the DPD approach. SDPD is thermodynamically consistent, does not rely on arbitrary coefficients for its thermostat, involves realistic transport coefficients, and includes fluctuation terms. SDPD is implemented in our work for arbitrary 3D geometries with a methodology to model solid wall boundary conditions. We present simulations for isothermal flows for verification of our approach. The entropy equation is implemented with a velocity-entropy Verlet integration algorithm Flows with heat transfer are simulated for verification of the SDPD. We present also the self-diffusion coefficient derived from SDPD simulations for gases and liquids. Results show the scale dependence of self-diffusion coefficient on SDPD particle size

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