Abstract Submitted
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Mesoscopic modeling of non-isothermal fluid systems[1] ZHEN LI, YUHANG TANG, Division of Applied Mathematics, Brown University, BRUCE CASWELL, School of Engineering, Brown University, GEORGE EM KARNIADAKIS, Division of Applied Mathematics, Brown University — The dynamical properties of fluid, including diffusivity and viscosity, are temperature-dependent and can significantly influence the flow dynamics in non-isothermal systems. To capture the correct temperature-dependence of a fluid, an energy conserving dissipative particle dynamics (eDPD) model is developed by expressing the weighting functions of the dissipative force and the random force as functions of temperature. The diffusivity and viscosity of liquid water at various temperatures ranging from 273K to 373K are used as examples for verifying the proposed model. For non-isothermal fluid systems, the present model can predict the diffusivity and viscosity consistent with available experimental data of water at various temperatures. Moreover, an analytical formula for determining the mesoscopic heat friction is proposed. The validation of the formula is confirmed by reproducing the experimental data in Prandtl number of liquid water at various temperatures. The proposed method is demonstrated in water but it can be readily extended to other liquids.

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