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Modeling of advection-diffusion-reaction processes using transport dissipative particle dynamics[1] ZHEN LI, ALIREZA YAZDANI, Division of Applied Mathematics, Brown University, ALEXANDRE TARTAKOVSKY, Computational Mathematics Group, Pacific Northwest National Laboratory, GEORGE EM KARNIADAKIS, Division of Applied Mathematics, Brown University — We present a transport dissipative particle dynamics (tDPD) model for simulating mesoscopic problems involving advection-diffusion-reaction (ADR) processes, along with a methodology for implementation of the correct Dirichlet and Neumann boundary conditions in tDPD simulations. In particular, the transport of concentration is modeled by a Fickian flux and a random flux between tDPD particles, and the advection is implicitly considered by the movements of Lagrangian particles. To validate the proposed tDPD model and the boundary conditions, three benchmark simulations of one-dimensional diffusion with different boundary conditions are performed, and the results show excellent agreement with the theoretical solutions. Also, two-dimensional simulations of ADR systems are performed and the tDPD simulations agree well with the results obtained by the spectral element method. Finally, an application of tDPD to the spatio-temporal dynamics of blood coagulation involving twenty-five reacting species is performed to demonstrate the promising biological applications of the tDPD model.

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