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**Modeling Material Diffusion in Combustion Processes Using Smoothed Dissipative Particle Dynamics** NIKOLAI PETSEV, XIA MA, BRYAN HENSON, BRAD CLEMENTS, Los Alamos National Laboratory — We describe a novel mesoscale particle-based strategy for modeling material diffusion in combustion processes. Importantly, this simulation framework gives the foundation for investigating the deflagration-to-detonation transition (DDT) in explosives, where the material transitions from burning at a rapid subsonic pace (deflagration) to the emergence of a shockwave (detonation). The basis for this approach is "smoothed dissipative particle dynamics" (SDPD), a stochastic thermodynamically consistent strategy for solving the fluctuating hydrodynamic equations of Landau and Lifshitz. Presently our new approach incorporates heat and mass transfer driven by conduction and diffusion, exchange of heat and chemical species due to thermal fluctuations, and source terms arising from the chemical reaction. In future work, this will be coupled to the fluctuating momentum equation, or included in multiscale molecular-continuum simulations, opening the possibility for simulations studying DDT in energetic materials.

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