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Taming Fire at Microscale: Molecular Simulations and Devices for Microcombustion

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Combustion at the microscale is an attractive technology for mobile power generation with energy densities ~100 times higher than the current battery technology. Enabling microcombustion technology has been an elusive goal since 1990s. Conventional combustors cannot be scaled down directly due to fundamental limitations of length and time scales related to ignition time, thermal and viscous losses and radical quenching. New device concepts integrating microscale phenomena such as field-emission microplasma can significantly alter thermal and reaction processes for sustained microcombustion. The direct simulation Monte Carlo method allows to study combustion phenomena at the molecular level including state-to-state processes at conditions far from thermal equilibrium. The evolution of computational platforms and availability of highly scalable DSMC software open an opportunity for molecular simulations to enable improved microcombustion understanding, diagnostics and control. Such modeling is especially useful for combustion at high speeds and at the microscale due to nonequilibrium transport and chemistry. In this talk we review a framework for applying DSMC to model combustion at the molecular level and apply plasma and flow simulations for microcombustion devices. A modified DSMC chemical reaction framework is developed to ensure detailed balance and relaxation towards thermal equilibrium regardless of the internal energy relaxation rates. First, we consider a benchmark of H2–O2 premixed flame and compare with continuum modeling and experimental data. The DSMC simulations based on the extended framework are then applied for other combustion examples. We also consider a novel microcombustion device concept based on field-emission dielectric barrier discharge. Field emission based microplasma actuators generate highly positive space charge that can be used to preheat, pump and mix reactants in microscale geometries and offer a promising solution to the problems associated with initiating and sustaining microcombustion.