Abstract Submitted
for the DFD19 Meeting of
The American Physical Society

Simulation of combustion processes using the DSMC method[1]
SHREY TRIVEDI, R. STEWART CANT, JOHN K. HARVEY, University of Cambridge — A novel molecular simulation technique, namely the Direct Simulation Monte Carlo (DSMC) method, is used to simulate hydrogen-air combustion. This method uses simulation particles that represent a set of real molecules. These simulation particles emulate the motion of real molecules and their properties can be averaged to evaluate the bulk flow properties. The Quantum-kinetic (QK) model, which uses total collision energy, molecular dissociation energy, quantized vibrational energy levels and the principle of molecular reversibility, is employed to account for the reactions. A distinct advantage of DSMC is that, because of the use of molecular level simulations, it avoids using continuum Arrhenius reaction rates and simplified gradient laws for the diffusivities of mass, momentum and heat. One-dimensional and two-dimensional hydrogen-air flames are simulated using a detailed 21-step chemical scheme and the validation of the properties of these flames is provided using the standard results in the literature. DSMC is suggested as an effective tool to provide the reaction rates and more importantly, the diffusivities for more complex, lesser known combustion schemes.

[1]This work has been performed using resources provided by the "Cambridge Service for Data Driven Discovery" (CSD3, http://csd3.cam.ac.uk)

Shrey Trivedi
University of Cambridge

Date submitted: 31 Jul 2019 Electronic form version 1.4