Abstract Submitted
for the DFD12 Meeting of
The American Physical Society

The Effect of Rotational Non-equilibrium on Chemical Reaction Rates Predicted by the Quantum-Kinetic (Q-K) Model for Direct Simulation Monte Carlo (DSMC) Simulations M.A. GALLIS, J.R. TORCZYNSKI, Sandia National Laboratories — The effect of non-equilibrium rotational excitation on dissociation and exchange reaction rates predicted by Bird's Q-K model is analyzed. The effect of rotational non-equilibrium is introduced as a perturbation to the effect of vibrational non-equilibrium. For dissociation reactions, a small but measurable improvement in the rates is observed. For exchange reactions, the change is negligible. These findings agree with experimental observations and theoretical predictions. The results from one-dimensional stagnation-streamline and two-dimensional axi-symmetric DSMC implementations of the original and modified Q-K models are compared for a typical re-entry flow. The influence of rotational non-equilibrium in promoting chemical reactions is seen to be small for this type of flow. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Date submitted: 20 Jun 2012 Electronic form version 1.4