

Abstract Submitted
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DSMC Predictions of Chemical Reaction Rates between Atmospheric Species M.A. GALLIS, R.B. BOND, J.R. TORCZYNSKI, Sandia National Laboratories — A recently proposed chemical reaction model based solely on molecular-level information is applied to calculate equilibrium and non-equilibrium chemical reaction rates for atmospheric reactions in hypersonic flows. The DSMC model is capable of reproducing measured equilibrium reaction rates without using any macroscopic reaction-rate information. Since it uses only molecular-level properties, the new model is inherently able to predict reaction rates for arbitrary non-equilibrium conditions. The DSMC-predicted chemical reaction rates are compared to theoretically calculated and experimentally measured reaction rates for non-equilibrium conditions. The observed agreement provides strong evidence that molecular-level modeling of chemical reactions provides an accurate method for predicting equilibrium and non-equilibrium chemical reaction rates. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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