

Abstract Submitted
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The Quantum-Kinetic Chemical Reaction Model for Navier-Stokes Codes MICHAEL A. GALLIS, ROSS M. WAGNILD, JOHN R. TORCZYNSKI, Sandia National Laboratories — The Quantum-Kinetic chemical reaction model of Bird is formulated as a non-equilibrium chemical reaction model for Navier-Stokes codes. The model is based solely on thermophysical, molecular-level information and is capable of reproducing measured equilibrium reaction rates without using any experimentally measured reaction-rate information. The model recognizes the principal role of vibrational energy in overcoming the reaction energy threshold. The effect of rotational non-equilibrium is introduced as a perturbation to the effect of vibrational non-equilibrium. Since the model uses only molecular-level properties, it is inherently able to predict reaction rates for arbitrary non-equilibrium conditions. This ability is demonstrated in the context of both Navier-Stokes and DSMC codes. 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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