A HOLISTIC DSMC TRANSPORT DATABASE FOR RE-ENTRY AND ABLATION MODELING

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Abstract: Hybrid simulation frameworks combining Computational Fluid Dynamics (CFD) and Direct Simulation Monte Carlo (DSMC) are frequently employed to efficiently perform high-fidelity simulations of environments containing combined continuum/rarified flow. The use of DSMC, a stochastic, particle-based method, is necessary for high-Knudsen flow where continuum-based assumptions governing CFD break down. However, the DSMC methodology is generally very computationally inefficient to model the continuum regime. In a CFD/DSMC hybrid approach, obtaining an accurate, high-fidelity solution hinges on the consistent treatment of transport properties and the used thermochemical models employed within the two solvers. In principle, in regions where CFD and DSMC are both employed, the same gas mixture under the same conditions should have the same properties, regardless of simulation type. Observed differences should be due to non-equilibrium processes, rather than differences in physical models.

While the transport models governing CFD and DSMC simulations are starkly different, they can effectively be linked via their use of reduced Chapman-Enskog collision integrals. In CFD, these integrals are typically stored as fitted polynomial expressions and used to directly compute gas transport properties via mixing rules or the full Chapman-Enskog formulation [1]. In DSMC, they can be used to derive the collision parameters needed for the phenomenological collision cross-section models that govern particle interactions, via a Nelder-Mead optimization scheme [2].

The goal of this work is to provide a unified DSMC transport database encompassing the vast majority of known gas species encountered during atmospheric entry, on Earth or any other Solar System body. This goal is largely possible due to recently performed ab initio quantum chemistry calculations [3]. Combined with other high-fidelity literature sources, the planned database will consist of collision integral data for over 200 neutral and ionized species and over 17000 binary collisions. From these collision integrals, Nelder-Mead optimization is used to compute Variable Soft Sphere (VSS) collision model parameters for DSMC, fitted from 300 K to 20000 K. Initial comparisons of transport properties of relevant equilibrium gas mixtures show great agreement between CFD and DSMC-derived results.

The completed database can be readily applied to model binary collisions of any gas mixture containing the included species over the specified temperature range, making it a valuable tool for future planetary probe modeling efforts. An example is shown below. Equilibrium mixture transport properties for a 19-species Titan atmospheric model [4] are computed using both fitted VSS parameters and the original CFD collision integral values. Deviations in computed properties between the two approaches are less than 5% for the entire temperature range.

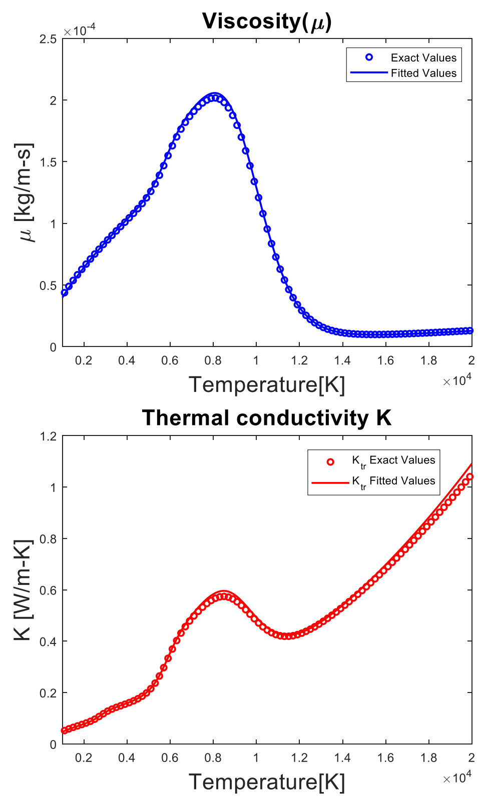

Figure 1: Equilibrium Mixture Properties for Titan (Initially 97% N2, 2.3% CH4, 0.7% Ar)

References:

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