Recommended DSMC Collision Model Parameters for Planetary Entry

M. R. Gosma[1], K. Swaminathan Gopalan[2], and K. A. Stephani[1,a)]

[1] *Center for Hypersonics and Entry Systems Studies, Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL, 61801*
[2] *Analytical Mechanics Associates Inc, NASA Ames Research Center, Mountain View, CA, 94043*

[a)] Corresponding author: ksteph@illinois.edu

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 consisting of both continuum and rarified flow. DSMC is a stochastic, particle-based method which solves the fundamental Boltzmann equation and is therefore necessary for high-Knudsen flow where continuum-based assumptions governing CFD break down. However, the DSMC methodology is generally 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 thermo-chemical 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.

The goal of this work is to provide a comprehensive DSMC transport database encompassing the vast majority of known gas species encountered during Earth or other planetary atmospheric entry. This goal is largely possible due to recently performed *ab initio* quantum chemistry calculations [1]. Combined with other high-fidelity data, the planned database will consist of collision integral data for over 200 neutral and ionized species and over 20000 binary collisions. From these collision integrals, Nelder-Mead optimization [2] is used to compute *collision-specific* Variable Soft Sphere (VSS) collision model parameters, 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 in Fig. 1. Equilibrium mixture transport properties for a 35-species mixture [3] composed originally of 10% air and 90% pyrolysis species of a carbon-phenolic ablator material [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.

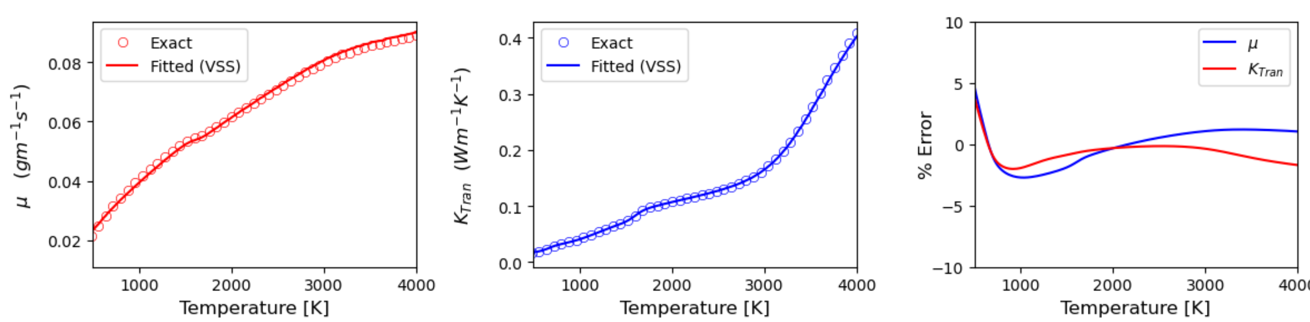

Fig. 1. Equilibrium TACOT Pyrolysis Gas – Air Mixture [3] (C:6, H:6, O:1.4, N:1.6)

ACKNOWLEDGEMENTS

This work was supported by a NASA Space Technology Graduate Research Opportunity (NSTGRO) Fellowship.

REFERENCES

[1] G. Bellas Chatzigeorgis, *Physics of Fluids*, **34**, 087106 (2022).
[2] K. A. Stephani, *Physics of Fluids*, **24**, 077101 (2012).
[3] A. Bellemans, *Physics of Fluids*, **31**, 096102 (2019).
[4] J. Lachaud, *Int. J. Heat Mass Transfer*, **90,** 1034-1045 (2015).