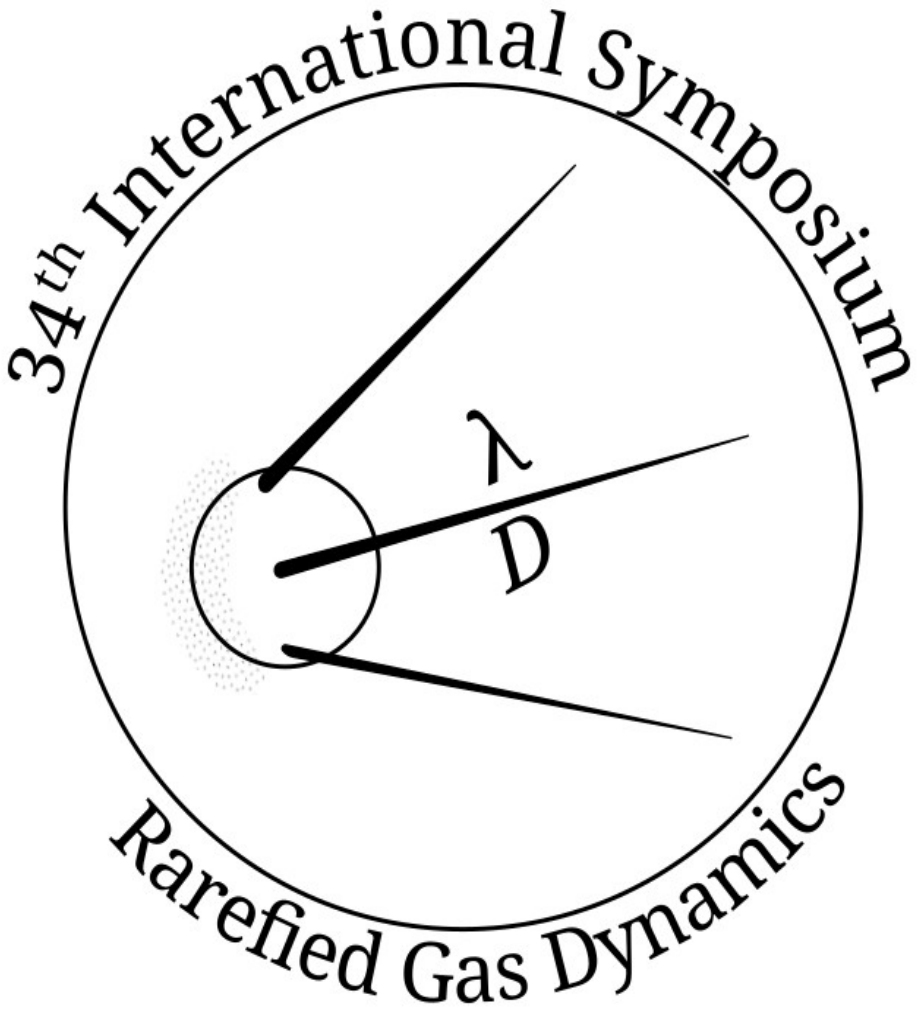


34th International Symposium on Rarefied Gas Dynamics

Brisbane, Australia, 13th to 17th July, 2026

Book of Abstracts

Gas Surface Interaction Model for Very Low Earth Orbit (VLEO) Systems

A. Appar[1,a)] and S. J. Poovathingal[2]

[1]*Department of Aerospace Engineering, Universidad Carlos III de Madrid, Leganés, 28911, Madrid, Spain.*
[2]*Department of Mechanical and Aerospace Engineering, University of Kentucky, Lexington, 40506, KY, USA.*

[a)]Corresponding author: ahilan.appar@uc3m.es

Accurate estimation of the drag force is essential for spacecraft in a very low Earth orbit (VLEO), as it significantly impacts orbit prediction, control, and collision avoidance. Accurate gas–surface interaction (GSI) models are crucial for predicting drag, particularly in collisions involving hyperthermal atomic oxygen (AO) with spacecraft surfaces operating in VLEO environments. This work examines the scattering of AO on amorphous silica, a common satellite material, using reactive molecular dynamics (MD). A comparison of angular scattering distributions and energy transfer between MD calculations and molecular beam experiments reveals excellent agreement [1]. Based on the physical insights from molecular dynamics calculations, a new hybrid GSI model has been developed [2]. The new model, termed the diffuse–Cercignani–Lampis–Lord (DCLL) model, combines velocity contributions from non-drifting diffuse Maxwellian and impulsively scattering drifting distributions. The new model reproduces angular flux distributions observed in molecular dynamics and beam experiments, while preserving a structure suitable for implementation into particle solvers such as direct simulation Monte Carlo (DSMC) and test particle Monte Carlo (TPMC). The DCLL model is both simple and accurate, effectively bridging molecular-level fidelity with practical usability and providing a reliable tool for drag prediction and orbital analysis of VLEO spacecraft.

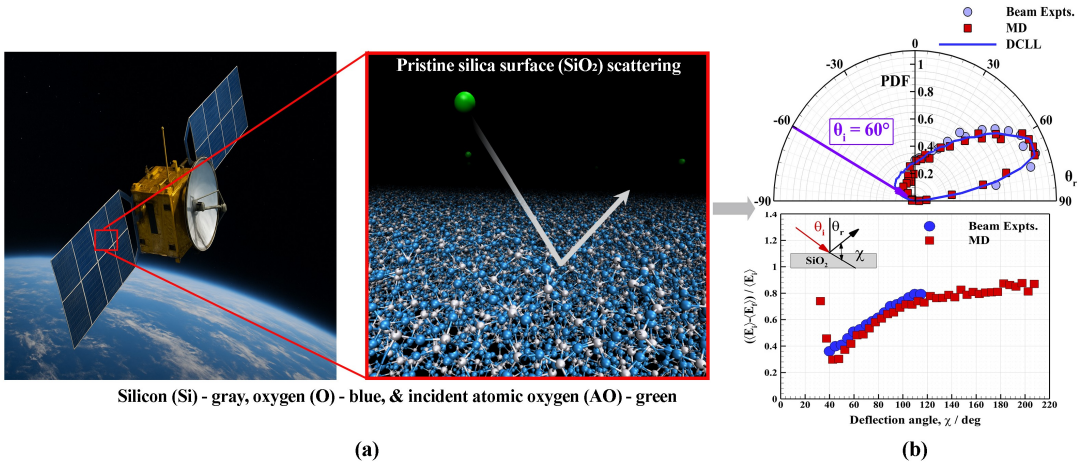


Fig. 1. (a) Schematic representation of GSI on a VLEO satellite surface. The magnified view illustrates the MD scattering simulation of atomic oxygen on a silica surface. (b) Validation of post-scattering data from MD with beam experiment and construction of a new GSI model (DCLL).

ACKNOWLEDGEMENTS

The material is based upon the work supported by the DARPA Young Faculty Award #D24AP00309 to Poovathingal. The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of DARPA or the U.S. Government. The U.S. Government is authorized to reproduce and distribute reprints for Government purposes, notwithstanding any copyright notation hereinafter. Resources supporting this work were provided by the NASA High-End Computing (HEC) Program through the NASA Advanced Supercomputing (NAS) Division at Ames Research Center. We also thank the University of Kentucky Center for Computational Sciences and Information Technology Services Research Computing for their support and use of the Morgan Compute Cluster and associated research computing resources.

REFERENCES

[1] A. Goto, P. D. Jorge, C. Xu, I. Gouzman, T. K. Minton, *ACS App. Poly. Materials.,* **7** (2025).
[2] A. Appar, S. J. Poovathingal, *Aerospace Science and Technology,* 111550 (2025).

Construction of a Unified Gas-Kinetic Wave-Particle Method for ES-BGK Models

Céline Baranger[1,a)], Alexis Copeau[1,2] and Luc Mieussens[2]

[1]*Bordeaux University, CNRS, Bordeaux INP, IMB*
[2]*CEA*

[a)]Corresponding author: alexis.coepeau@u-bordeaux.fr

The Unified Gas-Kinetic Wave-Particle method is a multiscale numerical approach for simulating gas flows over the entire range of Knudsen numbers, from highly rarefied to continuum regimes [1]. It can be viewed as a consistent hybridization of a stochastic particle solver for rarefied effects and a deterministic aerodynamic solver based on macroscopic wave propagations.

In rarefied regimes, nonequilibrium physics is resolved solely through discrete kinetic particles, leading to fast and accurate simulations. In the continuum regime, the method naturally degenerates into the Gas-Kinetic Scheme, acting as a standard Navier-Stokes solver with high efficiency. Finally, in the transitional regime, kinetic particles and aerodynamic waves contribute simultaneously in adaptively proportion, enabling an efficient and faithful representation of the interactions between continuous aerodynamic waves and rarefaction effects.

While the UGKWP method has been extensively validated for BGK, Shakhov and Rykov models [2], this work focuses on its extension to recent polyatomic Ellipsoidal-Statistical BGK models accounting for rotational and vibrational energy modes [3, 4]. The construction of the method is detailed, and its validity is assessed through numerical comparisons with reference solvers from the literature, including SPARTA [5] for non-vibrating gas flows, PICLas for other cases as it can handle polyatomic ES-BGK models including vibrational phenomena [6] and a recent deterministic UGKS solver for ES-BGK models [7].

REFERENCES

[1] C. Liu, Y. Zhu, K. Xu, Journal of Computational Physics 401, 108977 (2020).
[2] X. Xu, Y. Chen, C. Liu, Z. Li, K. Xu, Journal of Computational Physics 442, 110496 (2021).
[3] Y. Dauvois, J. Mathiaud, L. Mieussens, European Journal of Mechanics - B/Fluids 88, 1Ž01316 (2021).
[4] J. Mathiaud, L. Mieussens, M. Pfeiffer, European Journal of Mechanics - B/Fluids 96, 65Ž01377 (2022).
[5] S. J. Plimpton, S. G. Moore, A. Borner, A. K. Stagg, T. P. Koehler, J. R. Torczynski, M. A. Gallis, Physics of Fluids 31, 08610108 (2019).
[6] M. Pfeiffer, Physics of Fluids 30, 11610311 (2018).
[7] C. Baranger, A. Coepeau, L. Mieussens, Proceedings of the 3rd International Conference on Flight vehicles, Aerothermodynamics and Re-entry (FAR 2025) 232Ž013239 (2025).

Residual Closure of Navier-Stokes-Fourier System for Rarefied Flows

Y. Wang[1,a)], H. Gorji[2] and P. Jenny[1]

[1]*E.T.H. Zurich, Switzerland*
[2]*EMPA*

[a)]Corresponding author: yijwang@student.ethz.ch

Multiscale modeling plays a central role in modern science and engineering and remains one of the most challenging tasks. A prominent example in fluid dynamics is the description of flows in the near-continuum regime, where solvers based on accurate kinetic models become prohibitively expensive to solve, while the Navier-Stokes-Fourier (NSF) system is no longer valid. We present a novel approach to this problem by augmenting the NSF equations with a residual source term that accounts for the discrepancy between the continuum and kinetic models. The residual term is closed using a nonlinear super-stencil (NLSS), a compact stencil that extracts macroscopic flow data and maps them to the residual source term through a neural network. Boundary conditions incorporating velocity slip and temperature jump effects are likewise predicted by the NLSS framework. We apply the proposed method to planar channel flows and demonstrate that, using limited training data spanning only ranges of Knudsen and Mach numbers, the model accurately predicts previously unseen flow conditions, including cases with walls at different temperatures and moving at different velocities. These results demonstrate the strong potential of the proposed approach for modeling fluid flows beyond the continuum regime at the efficiency of continuum formulations. More broadly, the methodology offers a general framework for multiscale modeling across a wide range of physical systems.

Physics-Informed Neural Particle Method for the Spatially Homogeneous Landau Equation

M. Kim[1,a)], Y. Kim[1], D. Lee[2] and S-J. Son[2]

[1]*Seoul National University of Science and Technology*
[2]*Pohang University of Science and Technology*

[a)]Corresponding author: sungjun129@postech.ac.kr

In this work, we propose a novel neural-network-based framework for particle methods commonly used in gas dynamics and fluid mechanics. While classical particle methods track the time evolution of particles using explicit time-stepping schemes such as the Euler or fourth-order Runge2̌013Kutta (RK4) methods, we demonstrate that particle trajectories can instead be approximated through Physics-Informed Neural Networks (PINNs). Moreover, motivated by the score-based formulation underlying kinetic equations, we approximate the score function by an additional neural network and couple it with the network that learns particle trajectories. This results in an interacting two-network architecture, where the learned score function guides the evolution of particles while the particle dynamics, in turn, inform the score approximation. Through this coupled framework, we aim to approximate solutions of the spatially homogeneous Landau equation at the particle level. The proposed approach combines the interpretability of particle-based numerical methods with the flexibility of neural network approximations, providing a scalable and flexible alternative to conventional time-integration schemes for kinetic equations.

Aerobraking and Professor Kojiro Suzuki: Contributions and Legacy

M. Berthet[1,a)]

[1]*Graduate School of Engineering, The University of Tokyo, Hongo 7-3-1, Bunkyo-ku, Tokyo, Japan*

[a)]Corresponding author: berthet@daedalus.k.u-tokyo.ac.jp

Aerobraking is a type of manoeuvre in a rarefied planetary atmosphere. A spacecraft uses aerodynamic drag to progressively circularise its orbit, over tens or hundreds of atmospheric passes. The spacecraft's orbital energy is slowly reduced via collision with atmospheric gas particles, typically in the transitional flow regime. Aerobraking presents both engineering and scientific interest, since it enables drastic reduction in propellant mass compared to purely propulsive orbit transfer, and its fundamental mechanism is reliant on rarefied gas dynamics. This compelling combination of space mission engineering and rarefied flow physics may explain why aerobraking drew the attention of the late Professor Kojiro Suzuki [1, 2]. In fact, early in his career, Professor Suzuki contributed to the very first aerobraking mission, Hiten, by investigating the cause of apparent discrepancy between measured and predicted aerodynamic heating during aerobraking at Earth [3]. Over the ensuing decades, spacecraft aerodynamics in the upper atmosphere has remained one of Professor Suzuki's core interests, which he has transmitted to the wider community through teaching, supervision, collaborative research, outreach, and leadership in scholarly organisations. This paper overviews some of Professor Suzuki's major contributions to the field, with a focus on aerobraking, and introduces recent work being done in collaboration with the author, towards small satellite aerobraking.

ACKNOWLEDGEMENTS

The research was financially supported by a Japan Society for the Promotion of Science (JSPS) Grant-in-Aid for Early-Career Scientists, Project Number 24K17444. The paper is dedicated to Professor Kojiro Suzuki, who passed away in December 2024.

REFERENCES

[1] K. Yamada, *Aeronautical and Space Sciences Japan* **73**, 254–256 (2025), (in Japanese).
[2] M. Berthet, K. Yamada, E. Rathakrishnan, M. Lobbia, K. Fujita, *Journal of Evolving Space Activities* (2026), (accepted, in press).
[3] T. Abe, K. Suzuki, J. Kawaguchi, *Proceedings of the IUTAM Symposium on Aerothermochemistry of Spacecraft and Associated Hypersonic Flows* (Marseille, France, 1992), 21–26.

Abstract 13

DSMC coupling with peridynamics for aero–thermal–structural analysis

S. W. Hu[1], X. Wang[1,2], Y. Wang[1], G. Zhang[1], T. B. Xiao[1,3], and **Y. H. Zhang**[1,3a]

[1] *Centre for Interdisciplinary Research in Fluids, Institute of Mechanics, Chinese Academy of Sciences, Beijing, China.*
[2] *School of Future Technology, University of Chinese Academy of Sciences, Beijing, China.*
[3] *School of Engineering Science, University of Chinese Academy of Sciences, Beijing, China.*

[a)] Corresponding author: yonghao.zhang@imech.ac.cn

Accurate prediction of aerodynamic heating is essential for the reliable design of thermal protection systems. In high-enthalpy non-equilibrium flows, transient surface temperature directly regulates finite-rate surface chemistry and feeds back into local heat flux. However, the conventional decoupled approaches neglect this feedback and heat conduction within solid surface material. Moreover, the influence of pre-existing structural discontinuities (such as cracks) on aerothermal response remains largely unexplored.

To address these research challenges, we propose a coupled computational framework integrating the direct simulation Monte Carlo (DSMC) method with the bond-based peridynamics (BBPD) method [1], where DSMC resolves non-equilibrium gas–surface interactions and finite-rate surface chemistry while BBPD describes heat conduction in solid materials and material discontinuities. This strong coupling allows us to simulate gas flow, surface reaction, and thermal diffusion simultaneously.

A systematic aero–thermal–structural analysis reveals a wall-temperature-dependent competition between heat convection and energy generated by surface chemical reaction. Neglecting heat conduction within the surface material leads to distorted wall temperature distribution thus inaccurate predictions of chemical reaction and species depletion, see Fig. 1. Furthermore, the structural discontinuity at cracks causes thermal induction barrier, which inhibits inward heat conduction and triggers local temperature surge. The temperature spike intensifies surface catalysis and rapidly accumulates chemical heat to form localized hotspots.

The proposed DSMC-PD hybrid model uniquely enables simultaneous simulation of gas flow, surface chemistry and heat conduction within surface materials. In addition, this model is able to deal with material defects including cracks. Therefore, it enables a useful tool to accurately assess aerothermal loads and surface response.

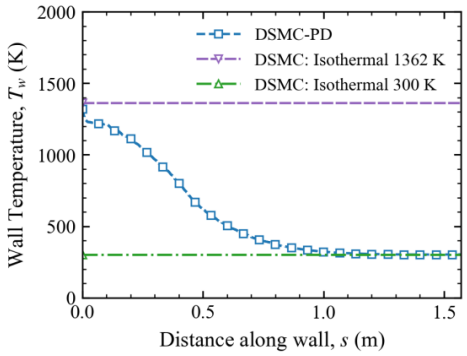


Fig. 1. Comparison of the surface temperature of a cylinder, where *s* is the distance from the stagnation point.

REFERENCES

[1] S. A. Silling, *Journal of the Mechanics and Physics of Solids* **48** (1) pp. 175-209 (2000).

Steady Solutions to the Relativistic Boltzmann Equation in a Slab

Jin Woo Jang[1,a)] and Seok-Bae Yun[1]

[1]*Department of Mathematics, POSTECH (Pohang University of Science and Technology), Cheongam-ro 77, Pohang, Gyeongbuk, Korea (37673)*
[2]*Department of Mathematics, Sungkyunkwan University, Seobu-ro 2066, Suwon, Gyeonggi, Korea (16419)*

[a)]Corresponding author: jangjw@postech.ac.kr

We study steady solutions to the relativistic Boltzmann equation with hard-sphere interactions in a slab geometry. Under a spatial symmetry assumption in the transverse variables x_2 and x_3, the problem reduces to a one-dimensional spatial slab $x_1 \in [0, 1]$ while retaining full three-dimensional momentum dependence. For non-negative inflow boundary conditions prescribed at $x_1 = 0$ and $x_1 = 1$, we prove the existence and uniqueness of a stationary solution in a weighted $L^1_p L^\infty_{x_1}$ framework, together with exponential decay in momentum.

Our analysis treats the full slab domain and does not rely on any smallness assumption on the slab width. We establish sharp coercivity and continuity estimates for the collision frequency, together with weighted convolution and pointwise bounds for the nonlinear gain term. These estimates generate and propagate a $(-\Delta_p)^{-1}$-type regularity within the solution framework, which plays a crucial role in the existence and uniqueness argument. In addition, we obtain uniform weighted integrability of the solution over arbitrary two-dimensional hyperplanes through the origin. This hyperplane estimate is derived as a genuinely *a posteriori* regularity property, without imposing any *a priori* hyperplane bounds, and follows from a Lorentz-invariant geometric reduction.

ACKNOWLEDGEMENTS

J. W. J. is supported by the National Research Foundation of Korea (NRF) grants RS-2023-00210484, RS-2023-00219980, 2022R1G1A1009044 and 2021R1A6A1A10042944. S.-B. Y. is supported by the National Research Foundation of Korea (NRF) grant funded by the Korean government (MSIT) (RS-2023-NR076676).

Nonequilibrium Hydrogen Kinetics for Gas Giant Atmospheric Entry

Clément H. B. Civrais[1,a)], Sung Min Jo[2] and Marco Panesi[1]

[1]*Department of Mechanical and Aerospace Engineering, University of California, Irvine, CA 92697, USA.*
[2]*Center of Excellence in Hypersonics and Space Propulsion, University of Central Florida, Orlando, FL 32816, USA.*

[a)]Corresponding author: ccivrais@uci.edu

Gas giant planets present significant scientific potential for gaining insights into the formation of their rings and satellites, some of which may contain oceans, as well as for studying their magnetospheres and improving our understanding of atmospheric dynamics and composition. Indeed, the past two US planetary science decadal surveys [1, 2] have identified a mission to Gas Giant planets, i.e. Uranus and Neptune, as a priority flagship mission. This emphasis is further reinforced by the European Space Agency's Voyage 2050 programme [3], which highlights the importance of atmospheric entry missions to Gas Giant planets, which remain among the only planets in our Solar System yet to be explored. Several kinetic schemes for atmospheric entry into gas giants have been developed over the years. Although these schemes differ in their formulation, they consistently identify the dissociation of molecular hydrogen as the first kinetic process occurring during entry into a gas giant atmosphere, thereby requiring accurate characterisation. However, most existing schemes have been derived by extrapolating experimental measurements conducted at low temperatures to conditions relevant to gas giant atmospheric entry, leading to significant deviations from first-principles calculations [4].

The most common high-fidelity approach to gain physical insight into the kinetic processes of a reactive system consists of leveraging rovibrational-state-specific kinetic databases and integrating master equations (StS-ME), from which quantities of interest can be extracted, e.g. QSS rate coefficients, relaxation times and vibrational energy loss. This approach is deterministic, in that all internal states are treated as pseudo-species and their populations are tracked through a system of master equations. While this method provides a high level of detail on the underlying kinetic processes, the construction of rovibrational-specific kinetic databases for four-body reactive systems without assumptions is either computationally prohibitive or intractable. Specifically, for $H_2 - H_2$ collisions, each H_2 molecule may transition from one of 343 rovibrational states to any other, resulting in a total number of cross sections on the order of 10^9. Such a vast number of cross sections renders a fully resolved description intractable, unless assumptions and simplifications are introduced regarding the thermalisation of the collision partner.

A complementary approach for modelling detailed nonequilibrium chemistry is classical-trajectory calculation direct simulation Monte Carlo (CTC-DSMC), now more commonly referred to as direct molecular simulation (DMS) [5, 6]. The DMS method is an *ab initio* variant of the standard direct simulation Monte Carlo (DSMC) framework [7], in that it embeds first-principles trajectory calculations within the DSMC algorithm. In essence, DMS computes molecular trajectories on-the-fly as part of the simulation of an evolving gas. Rather than resolving all possible energy transitions, DMS selectively samples the most dominant transitions occurring with non-negligible frequency under the conditions of interest. Although computationally demanding, DMS has now become tractable for four-body reactive systems and multi-component gas mixtures.

The present work aims to revisit the kinetic scheme and gain physical insight into the energy-transfer and dissociative processes occurring during atmospheric entry into Gas Giant planets by means of DMS. The study involves performing DMS simulations across the full extent of Gas Giant atmospheres, enabling the characterisation of the driving kinetic mechanisms relevant to such missions. The solver is first verified through comparison with the StS-ME approach, using the recently developed rovibrational state-specific kinetic database for the H_3 system [4], which allows for a direct comparison of the two methods without assumptions or simplifications. The DMS solver is then applied to resolve the full kinetics of the H_2 + H_2, H_2 + H, and H_2 + He systems under post-shock flow conditions relevant to Gas Giant entry missions.

REFERENCES

[1] National Research Council, *Vision and Voyages for Planetary Science in the Decade 2013-2022* (The National Academies Press, Washington, DC, 2011).
[2] National Academies of Sciences, Engineering, and Medicine, *Origins, Worlds, and Life: A Decadal Strategy for Planetary Science and Astrobiology 2023-2032* (The National Academies Press, Washington, DC, 2023).
[3] European Space Agency, "Voyage 2050: Long-Term Planning of the ESA Science Programme," Senior Committee Report (2021).
[4] H. Jeong, S. Jo, *AIAA SCITECH 2026 Forum* (Orlando, FL, AIAA Paper 2026-2644, 2026).
[5] T. E. Schwartzentruber, M. S. Grover, P. Valentini, *Journal of Thermophysics and Heat Transfer* **32**, 892–903 (2018).
[6] M. S. Grover, E. Torres, T. E. Schwartzentruber, *Physics of Fluids* **31**, 076107 (2019).
[7] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Oxford University Press Inc, 1994).

Multiscale Hybrid CFD/DSMC Simulation of Rocket-Induced Atmospheric Waves for Ionospheric Disturbance Prediction

G. K. Tavva[1,a)] and **G. W. Bowden**[2]

[1]*Department of Mechanical Engineering, BITS Pilani, Pilani Campus, Rajasthan 333031, India.*
[2]*School of Engineering and Technology, The University of New South Wales, Canberra ACT 2612, Australia.*

[a)]Corresponding author: gktavva@gmail.com

Exhaust plumes from launch vehicles expand to large dimensions at high altitudes, generating acoustic and gravity waves that propagate into the ionosphere as travelling ionospheric disturbances (TIDs). These disturbances are of interest for atmospheric diagnostics, remote sensing, and launch detection. However, linking plume dynamics to observed TID signatures remains challenging due to the multi-regime nature of the flow, which transitions from continuum conditions near the rocket to rarefied regimes in the upper atmosphere. This work presents a multistage hybrid simulation framework to model atmospheric wave generation by high-altitude rocket plumes. Building on the CFD–DSMC approach of [1, 2], which combined Ansys Fluent and SPARTA DSMC to capture shock structures in high-altitude Falcon 9 exhaust plumes, the present study introduces a staged coupling strategy that enables systematic propagation from the near-field plume to large-scale thermospheric interactions in 3-dimensions. The framework begins with a steady-state, two-dimensional axisymmetric CFD simulation of the near-field plume, assuming a thermally perfect viscous gas and neglecting chemistry, gravity, and rocket acceleration. A constant-collision-frequency surface is identified in a transitional region suitable for both continuum and DSMC descriptions and used as the interface for the next stage. Downstream, a medium-scale DSMC simulation resolves transitional and rarefied plume expansion, capturing molecular effects such as finite shock thickness and non-Maxwellian velocity distributions. The resulting solution provides boundary conditions for a final large-scale, three-dimensional DSMC simulation that resolves plume–atmosphere interactions and atmospheric wave generation in the stratified thermosphere. Coupling between the CFD and DSMC stages is achieved using MATLAB scripts. Preliminary results under representative launch conditions predict pressure and density perturbations consistent with observed ionospheric responses, demonstrating the framework's potential for physics-based prediction of launch-induced atmospheric waves.

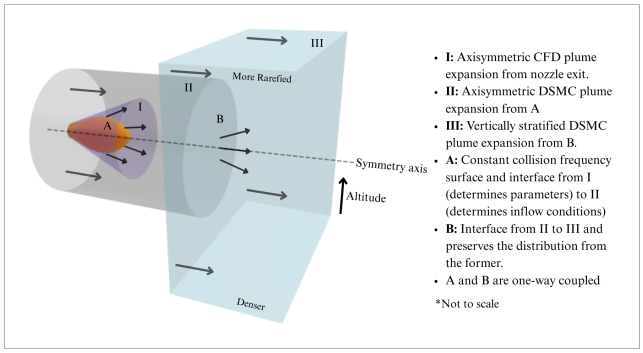


Fig. 1. 3D schematic of the computational domain under analysis.

ACKNOWLEDGEMENTS

The authors acknowledge institutional support from the University of New South Wales, Canberra. No external funding was received for this work.

REFERENCES

[1] G. W. Bowden, L. Pollock, M. Brown, *Proc. of the 24th Australasian Fluid Mechanics Conference* (Zenodo, Canberra, Australia, 2024), Paper ID–309.

[2] J. Papp, R. Wilmoth, C. Chartrand, S. Dash, *Proc. of the 42nd AIAA/ASME/SAE/ASEE Joint Propulsion Conference Exhibit* (AIAA, Sacramento, CA, USA, 2006), AIAA–2006–4412.

Physics-informed Neural Networks Based on the Fokker-Planck Model for Rarefied Gas Flows

Joonbeom Kim[1] and Eunji Jun[1,a)]

[1]*Department of Aerospace Engineering, Korea Advanced Institute of Science and Technology, 34141, Daejeon, Republic of Korea*

[a)]Corresponding author: eunji.jun@kaist.ac.kr

Rarefied gas flows in high-altitude atmospheres and in shock layers depart from local thermodynamic equilibrium, leading to the breakdown of continuum assumptions. The Direct Simulation Monte Carlo (DSMC) is a widely used particle-based method to describe such non-equilibrium flows. Although the DSMC method is applicable from rarefied to near-continuum regimes, its computational cost increases significantly near the continuum limit because particle collisions are more frequent. To address this limitation, the Fokker-Planck (FP) model was introduced, approximating the collision process as a drift-diffusion process in velocity space [1]. Advances in particle-based FP methods reduce computational cost compared with the DSMC method [2, 3], but statistical fluctuations due to particle sampling still remain. Deterministic methods, including the FP discrete-velocity method (FP-DVM), are another approach for solving rarefied gas flows [4]. The FP-DVM discretizes phase space and time, and solves the FP model on a discrete velocity grid using finite differences. While the FP-DVM avoids statistical fluctuations, maintaining accuracy requires a fine velocity-space grid and a large velocity domain, which results in high computational costs.

As a promising alternative to these traditional methods, physics-informed neural networks (PINNs) have gained attention for solving partial differential equations [5]. PINNs use a neural network to map spatiotemporal inputs to the solution fields of interest. During training, the network parameters are optimized by minimizing a loss function that includes the governing equations and boundary conditions. In this work, a PINN-FP model is proposed for rarefied gas flows, which integrates the FP equation into the loss function as a physics constraint. The proposed PINN-FP model predicts macroscopic moments up to the heat flux and reconstructs the velocity distribution function using Grad's 13-moment distribution function. Physics constraints are enforced by minimizing the velocity-space integrals of the FP equation residual, weighted by the 13-moment basis. These velocity-space integrals are evaluated using Gauss-Hermite quadrature. Figure 1 presents a schematic of the proposed PINN-FP model. The PINN-FP model provides continuous macroscopic moment fields, eliminates statistical fluctuations, and achieves high computational efficiency.

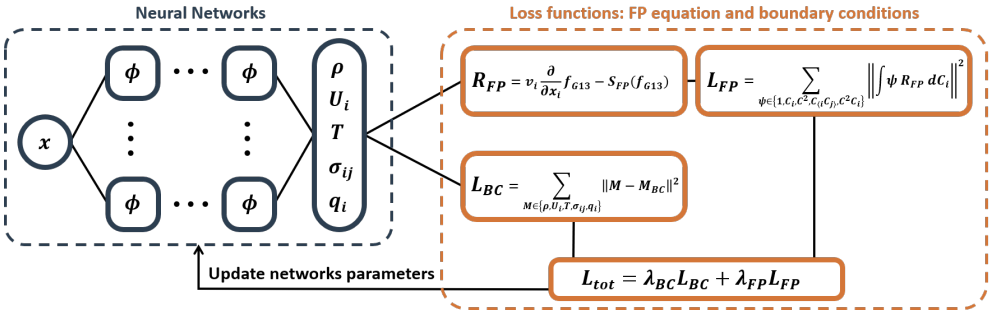


Fig. 1. Schematic of the PINN-FP model.

ACKNOWLEDGEMENTS

This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (RS-2025-00557012). This work was supported by the National Supercomputing Center with supercomputing resources including technical support(KSC-2025-CRE-0573).

REFERENCES

[1] J. Mathiaud, L. Mieussens, *Journal of Statistical Physics* **162**, 397–414 (2016).
[2] J. Kim, S. Kim, E. Jun, *Physics of Fluids* **36**, 127171 (2024).
[3] S. Kim, W. Park, E. Jun, *Computer Physics Communications* **304**, 109323 (2024).
[4] S. Liu, R. Yuan, U. Javid, C. Zhong, *Physical Review E* **100**, 033310 (2019).
[5] M. Raissi, P. Perdikaris, G. Karniadakis, *Journal of Computational Physics* **378**, 686–707 (2019).

Surface Roughness Effects on Gas–Surface Scattering and Recombination in VLEO

W. Park[1] and E. Jun[1,a)]

[1]*Department of Aerospace Engineering, Korea Advanced Institute of Science and Technology, Daejeon 34141, Republic of Korea*

[a)]Corresponding author: eunji.jun@kaist.ac.kr

Very Low Earth Orbit (VLEO) missions (150–400 km) offer distinct advantages for Earth observation and communications. However, satellites operating in VLEO experience significant aerodynamic drag due to increased atmospheric density and intense atomic oxygen (AO) flux. This environment necessitates accurate aerodynamic drag prediction under AO freestream conditions to ensure orbital sustainability.

Aerodynamic forces in VLEO are commonly predicted using the Direct Simulation Monte Carlo (DSMC) method, in which momentum transfer during gas–surface collisions plays a critical role. These collisions are governed by gas–surface interaction (GSI) models that describe both momentum scattering and surface chemical reactions. Consequently, uncertainty in DSMC-based aerodynamic predictions depends largely on the choice of GSI model. Previous studies have shown that specular gas–surface scattering results in lower aerodynamic drag than diffuse scattering, motivating efforts to increase surface specularity through the use of atomically smooth materials [1].

While specular gas–surface scattering and atomically smooth surfaces provide drag-reduction benefits, these advantages diminish over long mission durations under continuous exposure to high-energy ($\sim$ 5 eV) AO [2]. Sustained AO bombardment induces surface roughening and defect formation, leading to simultaneous changes in momentum scattering behavior and surface recombination characteristics. Previous studies have investigated the effects of surface roughness on scattering behavior and on recombination processes, but these investigations have generally been examined independently [3, 4]. As a result, existing GSI models remain limited in capturing VLEO conditions where surface degradation affects both aerodynamic and chemical surface interactions [5].

In this study, the effects of surface roughness on non-reactive scattering and reactive recombination are examined simultaneously, with surface roughness serving as the coupling parameter. Amorphous silicon dioxide (SiO_2) is employed as a representative AO-resistant surface material. Molecular Dynamics (MD) simulations with a reactive force field (ReaxFF) are used to evaluate GSI behavior over surfaces with varying roughness levels, and the resulting roughness-dependent GSI characteristics is incorporated into a DSMC framework. This approach offers a consistent framework for examining coupled aerodynamic and chemical effects under AO-induced surface degradation in VLEO.

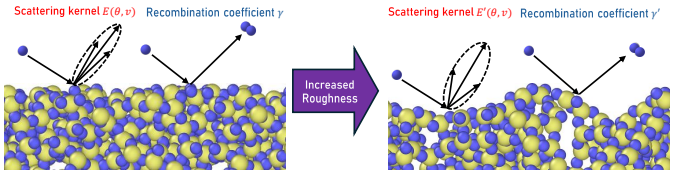


Fig. 1. Schematic illustraion of surface roughness effects on gas-surface interactions; yellow: Si, blue: O.

ACKNOWLEDGEMENTS

This work was supported by Korea Research Institute for defense Technology planning and advancement(KRIT) grant funded by the Korea government(DAPA(Defense Acquisition Program Administration)) (No. KRIT-CT-22-030, Reusable Unmanned Space Vehicle Research Center, 2026). This work was supported by the National Supercomputing Center with supercomputing resources including technical support(KSC-2025-CRE-0573).

REFERENCES

[1] T. K. Minton, T. E. Schwartzentruber, C. Xu, *ACS Applied Materials & Interfaces* **13**, 51673–51684 (2021).
[2] D. Khan, Y. Cho, J. R. Lee, H. Yoon, G. Park, J. G. Kim, *Aerospace Science and Technology* 110611 (2025).
[3] W. Park, E. Jun, *Physics of Fluids* **37** (2025).
[4] L. He, Z. Ye, Y. Cao, J. Tang, J. Zhao, D. Wen, *Physics of Fluids* **35** (2023).
[5] S. Huh, G. Moon, E. Jun, *Aerospace Science and Technology* **158**, 109900 (2025).

Abstract 23

Kinetic Theory Analysis of a Lid-Driven Cavity Flow of a Gas: Behavior of the Gas near Sharp Corners

M. Hattori[1,a)]

[1] *Department of Aeronautics and Astronautics, Kyoto University, Kyoto 615-8540, Japan*

[a)] Corresponding author: hattori.masanari.4r@kyoto-u.ac.jp

A flow in a two-dimensional square cavity driven by a moving lid is a fundamental problem in fluid mechanics [1]. As corner-related properties, the Stokes equations under the no-slip condition predict an infinite series of Moffatt vortices near the lower corners, multivalued flow velocity at the upper corners, pressure and stress that diverge inversely with the distance from the upper corners, and infinite total forces acting on the lid and side walls [2]. The divergence of pressure, stress, and total forces imply, at least locally, difficulties in describing the lid-driven cavity flow using conventional fluid mechanics. Considering a monatomic gas as a fluid, we can estimate that the fluid-dynamic description would break down within a mean-free-path-scale region near the upper corners. Kinetic theory may give a more reliable description for such a situation.

There are several kinetic-theory studies on the lid-driven flow in a rectangular cavity in the past two decades (see, e.g., Refs. [3, 4]). They commonly focus on non-equilibrium effects occurring in the bulk region. The magnitude of these effects is characterized by the Knudsen number, defined as the ratio of the mean free path of gas molecules to the size of the cavity.

While the characteristics of gas flows over a wide range of Knudsen numbers are analyzed in literature, investigations of the gas behavior near the corners have not been reported. In this context, a cavity flow, driven by a lid sliding *parallel* to its contact line with the cavity wall, was recently investigated as a first step in Ref. [5]. This setting is simpler than the conventional cavity flow and the corner singularity of interest arises regardless of the direction of lid motion. Owing to this simplification, Ref. [5] demonstrated that, in contrast to the conventional fluid-dynamic description, both the stress and total force acting on the surfaces remain finite within kinetic theory. However, in the setting, due to the direction of lid motion, only the shear stress components are nonzero and the flow is unidirectional. Pressure variations and vortices do not manifest themselves. As the flow strongly depends on the direction of lid motion, the analysis in the original setting is desirable.

Thus, in the present work, we consider a steady gas flow in a square cavity driven by a lid sliding *perpendicular* to its contact line (see also Fig. 1). The problem is formulated using the linearized Bhatnagar–Gross–Krook equation and the diffuse reflection boundary condition and reduced to a system of linear integral equations for macroscopic quantities, which is advantageous for accurate numerical analysis. Based on the numerical results for small Knudsen numbers, the following points are clarified. For Knudsen numbers larger than a threshold of $O(0.01)$, only a primary vortex exists and no corner vortices appear. Below this threshold, corner vortices appear, and their number is finite for each Knudsen number. Macroscopic quantities, including the flow velocity, are multivalued also within kinetic theory. For moderate to large Knudsen numbers, multivaluedness manifests itself even at the lower corners. The stress and pressure vary inversely with the distance from the upper corners up to a few tens of mean free paths. Their increase is suppressed at positions closer to the corners and their magnitude remains bounded. Consequently, the total forces acting on the lid and side walls are also finite, and they exhibit an unconventional scaling Kn ln Kn for small Knudsen numbers Kn.

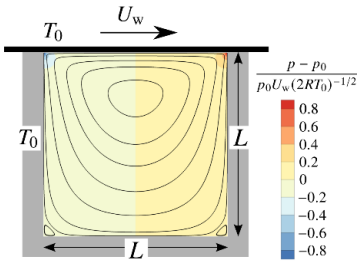


Fig. 1 Streamlines and pressure for $(\sqrt{\pi}/2)\mathrm{Kn} = 0.01$. [$\mathrm{Kn} = \ell_0/L$, ℓ_0: mean free path at equilibrium state with temperature T_0 and pressure $p_0 = \rho_0 R T_0$ (ρ_0: average density, R: specific gas constant)]

ACKNOWLEDGEMENTS

The present work was supported in part by JSPS KAKENHI grant no. 24K07302.

REFERENCES

[1] P. N. Shankar and M. D. Deshpande, *Annu. Rev. Fluid Mech.* **32**, 93–136 (2000).
[2] H. K. Moffatt, in *Lectures on Topological Fluid Mechanics* (Springer, Berlin, Heidelberg, 2009), pp. 157–166.
[3] S. Naris and D. Valougeorgis, *Phys. Fluids* **17**, 097106 (2005).
[4] L. Wu, J. M. Reese, and Y. Zhang, *J. Fluid Mech.* **748**, 350–367 (2014).
[5] M. Hattori, *Phys. Fluids* **36**, 052006 (2024).

Boundary conditions for fluid models describing neutral particles in the plasma edge of a fusion device

V. Maes[1,a)], W. Dekeyser[2], J. Koellermeier[3,4], M. Baelmans[2] and G. Samaey[1]

[1]*KU Leuven, Celestijnenlaan 200A, 3001 Leuven, Belgium.*
[2]*KU Leuven, Celestijnenlaan 300A, 3001 Leuven, Belgium.*
[3]*University of Groningen, Broerstraat 5, 9712 CP Groningen, the Netherlands.*
[4]*Ghent University, Sint-Pietersnieuwstraat 25, 9000 Gent, Belgium.*

[a)]Corresponding author: vince.maes@kuleuven.be

When simulating the behaviour of neutral particles in the plasma edge of a fusion device, typically a high-dimensional kinetic equation is solved that takes into account all kinds of interactions. At the boundary of the simulation domain, the equation is supplemented with boundary conditions that range from simple Dirichlet boundary conditions (representing, e.g., the density of neutrals disappearing deep in the plasma), to complex kernel based reflection boundary conditions at vessel walls [2]. Recently, a lot of work has been done to alleviate the high cost of kinetic neutral simulations by means of fluid and hybrid fluid-kinetic simulation strategies [1]. In this work, we investigate and compare different approaches to obtain suitable boundary conditions for the fluid neutral models that are being used in these strategies. First, we have Marshak-type boundary conditions that use the Maxwell approximation and do not resolve the boundary layer. Second, we have approaches that do resolve the boundary layer, at least approximately, such as the method of invariants, the source iteration method, and the method of moments. For each type of fluid boundary conditions, we discuss the used approximations and the effectiveness in reproducing the underlying kinetic boundary behaviour.

Numerical experiments for kinetic boundary conditions of inflow type and of reflection type are performed in a custom 1-dimensional C++ code. Reference solutions are calculated using a discrete velocity model (DVM). Testing the different fluid boundary conditions is done by supplementing them to the Hilbert expansion based fluid model from Ref. [3], and comparing the simulation results to those obtained by the DVM reference solver.

REFERENCES

[1] D. Borodin, F. Schluck, S. Wiesen, D. Harting, P. Börner, S. Brezinsek, W. Dekeyser, S. Carli, M. Blommaert, W. Van Uytven, M. Baelmans, B. Mortier, G. Samaey, Y. Marandet, P. Genesio, H. Bufferand, E. Westerhof, J. Gonzalez, M. Groth, A. Holm, N. Horsten, H. Leggate, *Nuclear Fusion* **62**, 086051August (2022).

[2] N. Horsten, "Fluid and Hybrid Fluid-Kinetic Models for the Neutral Particles in the Plasma Edge of Nuclear Fusion Devices," Ph.D., KU Leuven 2019.

[3] V. Maes, W. Dekeyser, J. Koellermeier, M. Baelmans, G. Samaey, *Physics of Plasmas* **30**June (2023), 10.1063/5.0146158, publisher: AIP Publishing.

Polyatomic chemistry modeling in DSMC using a harmonically-coupled-anharmonic-oscillator model

S. Lauterbach[1,a)], **F. Tuttas**[1,b)], S. Fasoulas,[1] and M. Pfeiffer[1]

[1]*Institute of Space Systems (IRS), University of Stuttgart, Pfaffenwaldring 29, 70569 Stuttgart, Germany*

[a)]Corresponding author: lauterbachs@irs.uni-stuttgart.de
[b)]Corresponding author: tuttasf@irs.uni-stuttgart.de

Atmospheric entry processes are characterized by high-enthalpy gas flows in strong thermal and chemical non-equilibrium. Accurate simulations of such conditions remain challenging due to the extreme conditions and the complex influence of internal energy modes. In particular, the common assumption of uncoupled harmonic vibrations may break down, and excited internal energy states can directly influence reaction rates. Previously an anharmonic oscillator model has been developed by Civrais et al. [1, 2] to improve the accuracy of the Direct Simulation Monte Carlo (DSMC) method [3] under such conditions. However, this extension has so far been limited to diatomic molecules.
For the DSMC implementation in the open-source gas and plasma code PICLas [4] a polyatomic chemistry model was developed, which explicitly considers anharmonic effects and intramolecular energy redistribution. Vibrational degrees of freedom are treated in a local mode basis [5], in which anharmonic stretching modes are harmonically coupled by harmonic bending modes. The coupling allows for the redistribution of localized vibrational excitation and thus permits to channel vibrational energy into different reaction pathways. Dissociation can occur by the strong excitation of a stretching mode, and specific modes can be coupled to the reaction coordinate of the transition state in bimolecular exchange reactions.
The newly developed model is evaluated by the comparison to high-fidelity calculations and experimental reaction rates under strong non-equilibrium conditions. Two representative processes are investigated: the dissociation of HCN, which exhibits a high degree of intramolecular vibrational energy redistribution, and the hydrogen-exchange reaction between methane and a hydrogen radical, in which only selected modes contribute to the reactive process.

ACKNOWLEDGEMENTS

This work is funded by the Deutsche Forschungsgemeinschaft project number 516238647 - SFB1667/1 (ATLAS - Advancing Technologies for Low-Altitude Satellites).

REFERENCES

[1] C. Civrais, C. White, R. Steijl, *Journal of Thermophysics and Heat Transfer* **37**, 534–548 (2023).
[2] C. Civrais, C. White, R. Steijl, *Physics of Fluids* **36** (2024).
[3] G. A. Bird, *Molecular gas dynamics and the direct simulation of gas flows* (Oxford university press, 1994).
[4] S. Fasoulas, C.-D. Munz, M. Pfeiffer, J. Beyer, T. Binder, S. Copplestone, A. Mirza, P. Nizenkov, P. Ortwein, W. Reschke, *Physics of Fluids* **31** (2019).
[5] M. Child, R. Lawton, *Faraday Discussions of the Chemical Society* **71**, 273–285 (1981).

Experimental Validation of Hydrogen Dissociation Schemes using Non-Equilibrium Uranus Entry Flow in the X2 Expansion Tube

D. Joslyn[1,a)], S. G. Lock[1], R. G. Watt[1], N. N. Gibbons[1], Y. Liu[1], R. G. Morgan[1] and C. M. James[1]

[1]*Centre for Hypersonics, School of Mechanical and Mining Engineering, The University of Queensland, St Lucia, QLD, 4072, Australia.*

[a)]Corresponding author: d.joslyn@uq.edu.au

The ice giants, Uranus and Neptune, are the least explored planets in our solar system, despite being archetypes for the most common class of exoplanet [1]. As a result, the most recent decadal survey for planetary exploration identified the Uranus Orbiter and Probe (UOP) as the current highest priority large flagship mission, initiating an influx of new chemical kinetics schemes for the modelling of its atmospheric entry [2]. Uranus' atmosphere contains mostly hydrogen and helium - a characteristic shared amongst the giant planets - but the hydrogen dissociation mechanism has been modelled poorly in the past. This mechanism was believed to be the main catalyst of uncertainty in existing radiative heating predictions for giant planet entry [3]. Accordingly, numerous hydrogen dissociation schemes have recently been proposed, but they are yet to be experimentally validated by a common source [4–6].

One method of quantifying dissociation is through spectroscopy, as it provides spatially-resolved species concentrations in the shock layer as they emit or absorb radiation. Molecular hydrogen emits bands of radiation, predominantly in the vacuum ultraviolet (VUV) wavelength region. Given the complexities surrounding the operation of VUV spectroscopy in impulse facilities, there is a lack of shock layer hydrogen bands quantified in literature. Simulating Uranus entry poses several other challenges, due to the extreme conditions required, at velocities above 20 km/s [3]. Combined, these key limitations affect the accuracy of hydrogen dissociation rates, as experimental validation is scarce.

The X2 expansion tube at the University of Queensland (UQ) is uniquely capable of providing the required validation case, utilising a VUV spectroscopy system for high-enthalpy planetary entry conditions. Currently, ice giant entry conditions require the test gas substitution method proposed by Stalker and Edwards [7]. Helium or neon is substituted in the test gas mixture to participate in heavy particle collisions, but not ionisation. The result is an increased post-shock temperature, but an unchanged density ratio. This allows the Uranus entry shock layer to be simulated and analysed, achieved with a reduced freestream velocity in the performance envelope of X2 [8].

The peak-velocity trajectory point during Uranus entry displays a significant region of non-equilibrium flow, such that hydrogen dissociation was observed across more than half of the shock layer in prior X2 experiments. Alongside strong H-α and Lyman-α lines, the H_2 Lyman band ($B^1\sum_u^+ - X^1\sum_g^+$) was substantial. Importantly, it was the only feature to obtain reasonable agreement with NEQAIR. However, these computational results relied on a simplified one-temperature CFD input, which employed the full Leibowitz and Kuo reaction rate scheme for a hydrogen/helium mixture [9].

The present work aims to detail the development and validation of an improved two-temperature hydrogen/helium model using UQ's compressible flow solver, Eilmer. The model may be used to simulate and compare the various hydrogen dissociation schemes available to date, maintaining the original Leibowitz and Kuo ionisation rates. Such outputs may be processed with NEQAIR to obtain the synthetic spectra from each case, where observations will be concentrated on the Lyman band in the VUV region. Finally, a comprehensive experimental validation against the emission spectroscopy from Uranus entry conditions in X2 will be undertaken, enabling the evaluation and comparison of the performance of each scheme.

REFERENCES

[1] L. N. Fletcher, *Planetary and Space Science* **191** (2020).
[2] K. E. Mandt, *Science* **379**, 640–642 (2023).
[3] B. A. Cruden, D. W. Bogdanoff, *Journal of Spacecraft and Rockets* **54**, 1246–1257 (2017).
[4] A. T. Carroll, G. Blanquart, A. M. Brandis, B. A. Cruden, *AIAA SciTech Forum* (2024).
[5] G. Colonna, L. Walpot, D. Ninni, F. Bonelli, G. Pascazio, L. D. Pietanza, A. Laricchiuta, *International Journal of Heat and Mass Transfer* **259** (2026).
[6] H. S. Jeong, T. W. Jeong, S. M. Jo, *AIAA SciTech Forum* (2026).
[7] R. J. Stalker, B. P. Edwards, *Journal of Spacecraft and Rockets* **35**, 729–738 (1998).
[8] C. M. James, D. E. Gildfind, R. G. Morgan, S. W. Lewis, T. J. McIntyre, *Journal of Spacecraft and Rockets* **57**, 656–671 (2020).
[9] L. P. Leibowitz, T. Kuo, *AIAA Journal* **14**, 1324–1329 (1976).

Development of a Particle Bhatnagar–Gross–Krook Method for Rarefied Monatomic Gas Mixtures

Inchan Kim[1], Joonbeom Kim[1], Woonghwi Park[1], and Eunji Jun[1,a)]

[1]*Department of Aerospace Engineering, Korea Advanced Institute of Science and Technology, Daejeon, 34141, Republic of Korea*

[a)]Corresponding author: eunji.jun@kaist.ac.kr

The Direct Simulation Monte Carlo (DSMC) method has long served as a reliable numerical approach for simulating rarefied and non-equilibrium gas flows. In DSMC, gas is represented as computational particles whose motion and collision is tracked stochastically. However, due to the strict cell size and time step constraints required to resolve individual binary collisions, its computational cost increases rapidly in near-continuum regimes. Kinetic modeling based on the Bhatnagar–Gross–Krook (BGK) framework offers a promising alternative [1]. By replacing the Boltzmann collision operator with a relaxation process toward equilibrium, the BGK framework alleviates the need to resolve individual binary interactions, making it computationally attractive in near-continuum regimes. Over the past few decades, numerous studies have aimed to develop BGK mixture models, motivated by the success of BGK models for single-species gases [2, 3]. To date, developing BGK mixture models have been pursued in two formulations: single-relaxation and multi-relaxation. Single-relaxation models employ a single effective relaxation by collapsing self-species and inter-species relaxation into a single mechanism. Although they show acceptable accuracy in many applications, capturing species pair-dependent relaxation processes is structurally limited. Multi-relaxation models, on the other hand, mimic the mixture Boltzmann collision operator, allowing pair-dependent relaxations. Despite being more physically grounded, the determination of transport properties is not fully resolved so far. Therefore, there is a clear need for a BGK mixture model that allows species pair-relaxation while preserving correct transport behavior.

Motivated by these limitations, we propose a new multi-relaxation BGK mixture model that ensures Navier–Stokes–Fourier (NSF) level transport behavior in the near-continuum regimes. The model adopts a multi-relaxation formulation that allows distinct relaxation processes for individual species pairs, while NSF-level transport is enforced by matching the production terms with those of the Boltzmann equation. Within this framework, the Unified-BGK (UBGK) equation, first introduced for single-species gases, is employed as the base model equation [4]. It provides four free parameters associated with momentum, energy, shear stress, and heat-flux relaxation, which are required for production-term matching. The resulting UBGK mixture model is implemented within SPARTA, an open-source DSMC solver developed by Sandia National Laboratories [5]. Validation for a supersonic flow around a cylinder demonstrates that the proposed UBGK mixture model accurately captures the temperature field and surface transport quantities, including heat flux and shear stress, with good agreement relative to DSMC reference solutions.

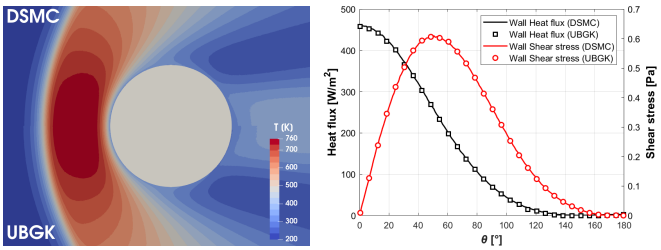


Fig. 1. Supersonic flow around a cylinder of a He–Ar–Kr mixture, Ma=3, Kn=0.02 (Left: Temperature contours around a cylinder; Right: Heat flux and shear stress profiles over the cylinder.)

ACKNOWLEDGEMENTS

This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (No. RS-2025-02213804). This work was supported by the National Supercomputing Center with supercomputing resources including technical support(KSC-2025-CRE-0573).

REFERENCES

[1] W. Park, S. Kim, M. Pfeiffer, E. Jun, *Physics of Fluids* **36**, 02711302 (2024).
[2] M. Pfeiffer, P. Nizenkov, S. Fasoulas, *AIP Conference Proceedings* **2132**, 10000108 (2019).
[3] M. Pirner, "Kinetic modelling of gas mixtures," Ph.D. thesis, Wurzburg University Press 2018.
[4] S. Chen, K. Xu, Q. Cai, *Advances in Applied Mathematics and Mechanics* **7**, 245–266 (2015).
[5] S. J. Plimpton, S. G. Moore, A. Borner, A. K. Stagg, T. P. Koehler, J. R. Torczynski, M. A. Gallis, *Physics of Fluids* **31**, 08610108 (2019).

Abstract 30

Vibrational Non-Equilibrium Effects on Rarefied Reactive Richtmyer-Meshkov Instability

W. A. Casseus [1] and **K. L. Pan**[1, a)]

[1] *Department of Mechanical Engineering, National Taiwan University, Taipei 10617, Taiwan*

[a)] Corresponding author: panpeter@ntu.edu.tw

The Richtmyer-Meshkov instability (RMI) [1] is a primary driver of mixing and ignition in supersonic combustion, yet the effects of thermal non-equilibrium on its evolution and on the subsequent combustion remain poorly understood [2]. This study investigates a microscale reactive RMI in a non-premixed H_2/O_2 gas pair, using a direct simulation Monte Carlo (DSMC) framework with a quantum-kinetic reaction model modified to preserve detailed balance [3]. We systematically characterize the competition between rarefaction, thermal relaxation, and chemical kinetics by controlling the pre-shock pressure to evaluate ignition performance in different high-altitude flight regimes. The results show that as rarefaction increases, RMI growth is prematurely arrested by the rapid increase in viscous dissipation, dampening the structures before non-linear mixing fully develops (Fig. 1). Moreover, non-equilibrium cases consistently reach a lower peak amplitude than equilibrium predictions, allowing less interfacial area for diffusive mixing to occur. Beyond its hydrodynamic impact, non-equilibrium effects fundamentally alter RMI-driven combustion, revealing a regime-dependent reversal in the rate of formation of H_2O (Fig. 2). At high pressure (1 atm), post-shock vibrationally cold conditions inhibit product formation as the system remains dominated by three-body chain-terminating reactions in that regime. Conversely, at low pressure (0.25 atm), these same conditions enhance product formation. This enhancement occurs because, at low pressure where three-body collisions are scarce, vibrationally cold states concentrate energy in translational modes, accelerating chain-branching through two-body reactions. These findings highlight the crucial role of non-equilibrium effects on local mixing and rarefied combustion, and suggest potential strategies for leveraging such regimes in high-speed propulsion systems at high altitude.

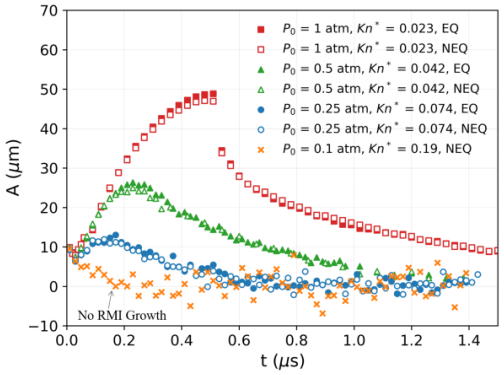


Fig. 1. Comparison plot of perturbation amplitude (A) evolution, where P_0 is the pre-shock pressure and Kn^* the post-shock Knudsen number.

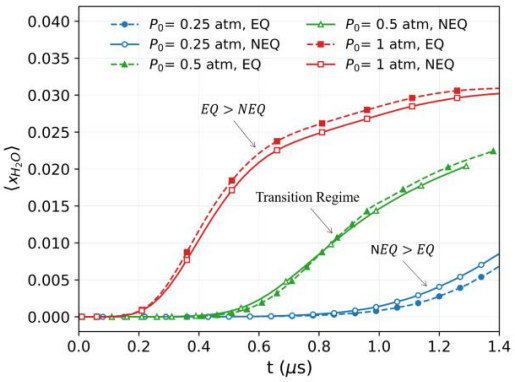


Fig. 2. Evolution of the average H_2O mole fraction for equilibrium (*EQ*) and non-equilibrium (*NEQ*) cases.

ACKNOWLEDGEMENTS

The work was supported by the National Science and Technology Council (NSTC) in Taiwan, through the project: NSTC-113-2221-E-002-188-MY2

REFERENCES

[1] R.D. Richtmyer, Taylor instability in shock acceleration of compressible fluids, *Comm. Pure Appl. Math*, 297-319, (1960).
[2] C. H. Chou, K. L. Pan, Computational investigation of chemical and non-equilibrium effects on the Richtmyer-Meshkov instability. *Proceedings of the Combustion Institute*, 40, 105335, (2024).
[3] C. H. Chou, K. L. Pan, Redistribution of the post-reaction internal energies in DSMC using quantum-kinetic model. *Computer Physics Communications*, 314, 109641, (2025).

Experimental investigation of the efficiency and compression ratio of a passive intake for air-breathing electric propulsion

J. Zorn[1,a)], M. Reinhardt,[1] and P.J. Klar[1]

[1]*Department of Experimental Physics I, Justus Liebig University Giessen, 35392 Giessen, Germany.*

[a)]Corresponding author: jana.zorn@physik.uni-giessen.de

The main challenges for realizing a functional air-breathing electric propulsion (ABEP) system are the design of the intake for collecting and compressing a sufficient amount of atmospheric residual gas used as propellant and a highly efficient thruster system for compensating the atmospheric drag.
Intake systems are often investigated with DSMC simulations [1]. However, one remaining challenge is the still unknown gas-surface interaction (GSI) between the approximately 8 km/s fast atomic oxygen and molecular nitrogen with the intake material. Designing an intake based on wrong assumptions concerning the underlying GSI will lead to mission failure. Typically either diffuse or specular reflection is assumed in the simulations. However, Minton et al. [2] measured the reflection of atomic oxygen with 8 km/s for different materials, and introduced a more accurate description of GSI using the CLL model. Nevertheless, this model is only a parametrization and the model parameters need to be determined based on experiments using the corresponding gas species of various velocities and the surface material taking into account its surface morphology.

In our experiment we will directly measure the efficiency and compression ratio of an passive, conically shaped intake, as shown in the experimental setup in Fig. 1. We will not attempt to recreate atmospheric conditions in this experiment, since we want to focus on the physical phenomena first. Therefore, an argon ion beam is generated by a radio-frequency ion thruster (RIT) as particle source in front of the intake. Various diagnostics, such as Faraday cups, retarding potential analyzers (RPA), and Langmuir double probes are being used to analyze the plume in front of the intake. Knowing the precise conditions in front of the intake will allow us to also perform simulations for different GSI using the same condition as in the experiment. Finally, the experimental and simulation results will be compared to validate the simulations and obtain a better understanding of the underlying GSI for an ABEP system, similar to that used in [3], but using an improved particle source and more diagnostics for the current experiment. Our results are a step towards optimizing ABEP systems based on a systematic comparison of theory and experiment.

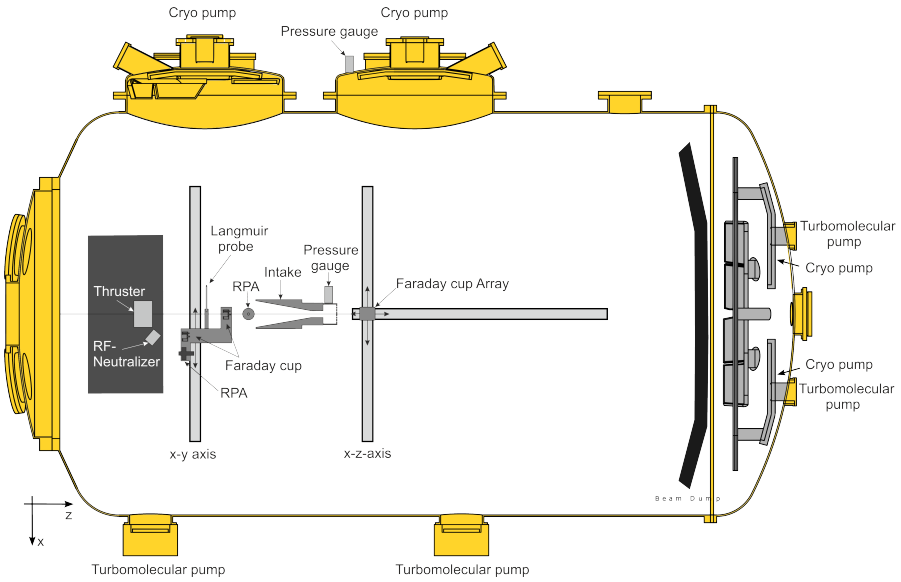


Fig. 1. Experimental setup used to investigate the performance of an passive intake for ABEP.

REFERENCES

[1] T. Andreussi, E. Ferrato, V. Giannetti, *Journal of Electric Propulsion* **1**, 31 (2022).
[2] T. Minton, T. Schwartzentruber, C. Xu, *ACS Applied Materials Interfaces* **13**, 43 (2021).
[3] J. Zorn, M. Reinhardt, K. Holste, P. Klar, *International Electric Propulsion Conference,* **IEPC-2025-194** (2025).

Investigation of Shock Standoff Distance in Hypersonic Rarefied Flows with DSMC Method

Wei Fang[1] and Zhi-Hui Wang,[1,2,a)]

[1]*School of Engineering Science, University of Chinese Academy of Sciences,101408, Beijing, PR China*
[2]*State Key Laboratory of Nonlinear Mechanics, Chinese Academy of Sciences, 100190, Beijing, PR China*

[a)]Corresponding author: wisdom@ucas.ac.cn

The shock standoff distance, denoted as Δ, represents a pivotal characteristic of flow field structures and plays a crucial role in aerodynamic and aerothermal computations [1, 2]. It also functions as a key parameter in theoretical models for predicting aerodynamic heating [3]. Previous extensive research has predominantly been confined to the field of continuum flows, focusing mainly on the thermochemical non-equilibrium effects under inviscid or high Reynolds number assumptions. However, new-generation near-space hypersonic vehicles, which frequently operate at high Mach numbers and moderate-to-low Reynolds numbers, fall within the domain of hypersonic rarefied flows. Inger [4] employed a zeroth-order Taylor series expansion of the continuity equation under the continuum assumption, demonstrating that the Δ can be regarded as a correction to the inviscid counterpart due to the boundary layer displacement thickness. This analysis also quantified the higher-order effects of vorticity and curvature on the Δ. However, the above theoretical evaluation still shows noticeable errors when applied to the Δ for the cylinders. This necessitates a deeper understanding of the shock standoff distance characteristics under hypersonic rarefied flow conditions.

In hypersonic and moderate-to-low Reynolds number flows, the presence of a boundary layer introduces two primary effects. On one hand, compared to an inviscid flow model, the lower mean velocity within the boundary layer leads to a displacement effect, which tends to increase Δ. On the other hand, the wall temperature at the leading-edge stagnation point is generally much lower than the freestream total temperature. The wall cooling effect increases the gas density near the wall, thereby reducing Δ. Consequently, a competitive mechanism arises between the viscous effects within the boundary layer and the wall cooling effects. In this paper, the direct simulation Monte Carlo (DSMC) method is employed to investigate the influence of hypersonic rarefied freestream conditions on the shock standoff distance. For freestream Reynolds numbers ranging from 10^3 to 10^4, the flow field can still be categorized into a layered structure that consists of an inviscid region and a viscous region, as illustrated in Fig. 1. Firstly, compared with the work of Inger [4], the present study performs a first-order Taylor series expansion of the continuity equation, thereby providing a clear physical interpretation of the higher-order effects quantified in previous studies. Secondly, the variation of Δ with *Re* is investigated under adiabatic conditions to eliminate wall cooling effects. Thirdly, the influence of wall temperature on Δ is analyzed for typical freestream conditions. By integrating these two competitive effects, the overall impact of the stagnation boundary layer on Δ in moderate-to-low Reynolds number flows is predicted. Finally, the generalizability of the current results is assessed by extending the analysis to more rarefied conditions, where the boundary layer and shock wave merge to form a shock layer.

This work quantitatively characterizes the variation of Δ in hypersonic rarefied flows, offering novel insights into the coupling mechanisms between viscous effects and wall cooling effects. The proposed correlation establishes a foundation for rapid engineering predictions of aerothermal environments in low Reynolds number flights.

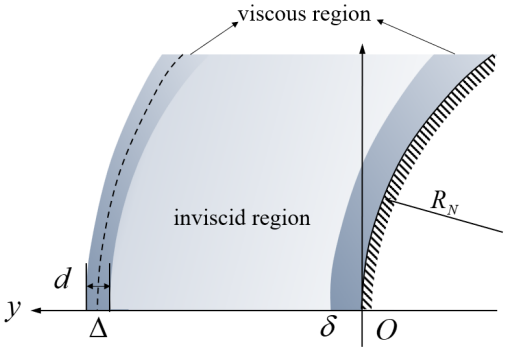


Fig. 1. Schematic diagram of the stagnation point flow and flow field structure behind a strong shockwave, where d, R_N, Δ, and δ represent the thickness of shockwave, the radius of curvature of the nose, the shockwave standoff distance, and the thickness of stagnation point boundary layer.

ACKNOWLEDGEMENTS

This work was supported by the Strategic Priority Research Program (B) of Chinese Academy of Sciences (grant XDB0620203).

REFERENCES

[1] R. Thakur, G. Jagadeesh, *Proceedings of the Institution of Mechanical Engineers, Part G: Journal of Aerospace Engineering* **231**, 2666–2676 (2017).
[2] N. Belouaggadia, H. Olivier, R. Brun, *Journal of Fluid Mechanics* **607**, 167–197 (2008).
[3] C. Wen, H. G. Hornung, *Journal of Fluid Mechanics* **299**, 389–405 (1995).
[4] G. R. Inger, *Journal of thermophysics and heat transfer* **18**, 108–113 (2004).

Abstract 33

Photophoretic force exerted on a membrane composed of rings.

Felix Sharipov[1,a)], Benjamin C. Schafer[2,3], Joost J. Vlassak[2]

[1] *Physics Department, Federal University of Parana, Curitiba-PR, Brazil*

[2] *John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge-MA, USA*

[1] *Rarefied Technologies Inc., Albuquerque-NM, USA*

[a)]Corresponding author: sharipov@fisica.ufpr.br

Recent studies [1,2] have shown that the photophoretic force acting on a perforated membrane is greater than that acting on a solid membrane, enabling the levitation of centimeter-scale membranes in near-space conditions. The adopted assumption in calculating photophoretic forces is that the pore size must be much smaller than the mean free path of gas molecules. However, fabricating porous membranes that satisfy this requirement remains challenging. As an alternative, membranes with periodic structures, such as grids with relatively large holes, can be considered. Such structures would be easier to fabricate and may serve as a practical substitute for porous membranes without significant loss of levitation performance. In this study, we compute the photophoretic force exerted on membranes with radially periodic geometries. Specifically, we investigate a circular membrane composed of multiple concentric rings. Two mechanisms of photophoretic force generation are considered. The first arises from a temperature difference between the top and bottom surfaces of the membrane, assuming identical surface properties on both sides. The second results from a difference in accommodation coefficients between the two sides of the membrane, while the membrane temperature is uniform but differs from that of the surrounding gas. The flow field and photophoretic force are calculated using the direct simulation Monte Carlo method based on *ab initio* interaction potentials. Gas–surface interactions with differing accommodation coefficients are modeled using the Cercignani–Lampis scattering kernel. In the complete version of this work, the influence of the number of rings on the photophoretic force will be reported. Comparisons with porous membranes indicate that a relatively small number of rings is sufficient to achieve comparable levitation forces. At present, experiments are being performed to validate the obtained theoretical results and to facilitate the fabrication of membranes to be used in near-space conditions.

REFERENCES

[1] F. Sharipov, B.C. Schafer, and D.W. Keith, *Phys. Fluids* **36**(8), 081707 (2024).

[2] B.C. Schafer, J. Kim, F. Sharipov, G-S Hwang, J.J. Vlassak, D.W. Keith, *Nature* **644**, 362-369 (2025).

Abstract 34

Pressure Profile along Microchannel induced by Thermal transpiration flow

H. Yamaguchi[1,2 a)], H. Kura[3], and I. Graur[4]

[1] *Department of Advanced Science and Technology, Toyota Technological Institute, 2-12-1 Hisakata, Tempaku, Nagoya, Aichi 468-8511, Japan.*
[2] *Department of Micro-Nano Mechanical Science and Engineering, Nagoya University, Furo-cho, Chikusa, Nagoya, Aichi 464-8603, Japan*
[3] *Department of Mechanical Systems Engineering, Nagoya University, Furo-cho, Chikusa, Nagoya, Aichi 464-8603, Japan*
[4] *Aix-Marseille Université, CNRS, IUSTI UMR 7343, 5 rue Enrico Fermi, 13453 Marseille, France.*

[a)] Corresponding author: hiroki@toyota-ti.ac.jp

Thermal transpiration flow is an interesting phenomenon in rarefied gas dynamics. Flow fields with temperature distributions commonly appear in practice, and it is important to understand this flow. Thermal transpiration has been studied for a long time, and the system with two reservoirs at different temperatures connected by a single channel has been investigated both numerically and experimentally to obtain the induced pressure difference, mass flow rate, and other flow characteristics. One of applications of this phenomenon is the Knudsen pump/compressor.

A few studies [1,2] have numerically shown pressure profiles inside a channel in the flow direction. These studies used a simple system consisting of a straight microchannel with different temperatures but the same pressure at both ends. Interestingly, the pressure was found to be not uniform along the channel. Specifically, an upward-convex profile was observed with a linear temperature distribution, whereas an upward-concave upward profile was obtained with an exponential temperature distribution.

In the present study, we kept the temperatures at both ends of the channel constant while slightly varying the temperature in the middle to induce a change in the curvature of the temperature profile. The effect of the curvature of the temperature profile on the resulting pressure profile along the channel was studied. In particular, the pressure variations at the middle of the channel were measured for the temperature profiles with different curvatures. Although these pressure variations along the channel were very small, the measured results were successfully verified by a numerical analysis.

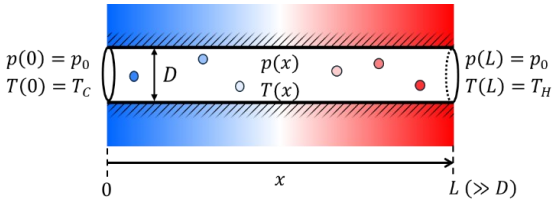


Fig. 1. A schematic of the measured microchannel with a thermal transpiration flow.

ACKNOWLEDGEMENTS

This work was partially supported by Grant for Basic Science Research Project from the Sumitomo Foundation Grant Number 210641, and JSPS KAKENHI Grant Number JP25K01171. The authors would like to thank Dr. Takehiro Hayasaka for his assistance with the laser microscope measurement.

REFERENCES

[1] I. Graur, F. Sharipov, *Microfluid. Nanofluid.*, **6**, pp. 267-275 (2009).
[2] M. Rojas-Cardenas, *Temperature Gradient Induced Rarefied Gas Flow* (Ph.D. thesis, Aix-Marseille University, 2012).

Model-Adaptive Simulation of Moment Models for Non-Equilibrium Gas Flows

Rik Verbiest[1] and Julian Koellermeier[1,2,a)]

[1]*University of Groningen, Broerstraat 5, 9712 CP Groningen, the Netherlands*
[2]*Ghent University, Sint-Pietersnieuwstraat 25, 9000 Gent, Belgium*

[a)]Corresponding author: j.koellermeier@rug.nl

In rarefied gases both near-equilibrium and non-equilibrium regions can exist simultaneously, which requires adaptive simulation methods to efficiently capture the varying levels of modeling complexity. One possibility is to use a higher-order moment model [1] for the non-equilibrium region and a lower-order moment model (or the Euler equations) for the near-equilibrium flow. In this setting, model adaptivity can leverage the hierarchical structure of moment models to enable an efficient and stable numerical simulation.

In this work, we present a model-adaptive numerical method for simulating one-dimensional rarefied gas flows modeled by the BGK equation [2] using the hyperbolic moment equations (HME) [3, 4] with space-dependent model order. The adaptive procedure consists of two main steps: (1) the domain decomposition into regions where different moment models should be used and (2) the spatial coupling between different moment models at the boundaries of the regions. In step (1), the domain is decomposed into subdomains, each modeled by a moment model of appropriate order, using as error indicators a combination of distribution-based and gradient-based criteria [5]. The distribution-based criterion reduces model order in regions where high-order moments are negligible, while the gradient-based criterion refines the model in regions with significant gradients in macroscopic quantities or moments. In step (2) a non-linear adaptation of the padded buffer cell approach [6] is proposed to couple moment models of different orders at their interfaces, ensuring stable integration across the different subdomains.

Our approach leverages the hierarchical structure of moment models, which allows the use of a single numerical solver throughout the whole domain, while using different models at the same time. The method is designed to efficiently capture non-equilibrium effects in rarefied gas flows, which means that a reasonably small model error is balanced with a fast runtime. The results of this work could be used to speed up simulations such as those encountered in high-altitude and atmospheric reentry scenarios, where the Knudsen number varies significantly.

Time permitting, we briefly outline how the results can be applied in other settings, e.g. for moment models of free-surface flows [7], or reduced order modeling based on machine learning [8, 9].

ACKNOWLEDGEMENTS

This work is part of the HiWAVE project with file number VI.Vidi.233.066 of the ENW Vidi research programme, funded by the Dutch Research Council (NWO).

REFERENCES

[1] M. Torrilhon, *Annual Review of Fluid Mechanics* **48**, 429–458 (2016).
[2] P. L. Bhatnagar, E. P. Gross, M. Krook, *Physical Review* **94**, 511–525 (1954).
[3] Z. Cai, Y. Fan, R. Li, *Communications on Pure and Applied Mathematics* **67**, 464–518 (2014).
[4] Y. Fan, J. Koellermeier, J. Li, R. Li, M. Torrilhon, *Journal of Statistical Physics* **162**, 457–486 (2016).
[5] J. Koellermeier, *AIP Conference Proceedings* **2132**, 12000408 (2019).
[6] R. Verbiest, J. Koellermeier, *accepted* .
[7] J. Kowalski, M. Torrilhon, *Communications in Computational Physics* **25**, 669–702 (2019), 1801.00046 .
[8] J. Koellermeier, P. Krah, J. Reiss, Z. Schellin, *Microfluidics and Nanofluidics* **28**, 16–16 (2024).
[9] A. Oriou, P. Krah, J. Koellermeier, *Machine Learning with Applications* **23**, 100850 (2026).

Molecular Dynamics Investigation of Aerodynamic Heating on Nano-Rough Surfaces in High-Speed Flows

Quan Han[1,2,a)], and Can Cao[2]

[1] *School of Mechanical and Electronic Engineering, Nanjing Forestry University, Nanjing 210037, China*

[2] *School of Mechanical Engineering, Southeast University, Nanjing 211189, China*

[a)] Corresponding author: quanhan@njfu.edu.cn

In high-altitude, high-speed vehicles, nanoscale gas-surface interaction (GSI) can strongly influence thermal management performance [1, 2]. Although macroscopic roughness typically intensifies aerodynamic heating by inducing flow separation and turbulence [3], the thermal role of nanoscale roughness is more subtle and remains comparatively underexplored. Here, molecular dynamics (MD) simulations are used to quantify the aerodynamic heating of randomly rough silicon carbide (SiC) surfaces subjected to a 1000 m/s argon flow. The results show that nanoscale roughness lowers the solid's steady-state temperature relative to an ideally smooth surface. Mechanistically, the gas-phase velocity distribution functions indicate preferential accumulation of argon atoms within surface valleys, forming a localized high-density near-wall layer. This near-wall layer acts as a kinetic energy sink by promoting intensified intermolecular collisions, so the kinetic energy of incoming particles is dissipated before reaching the solid lattice. This interpretation is consistent with the findings that the formation of an adsorbed layer increases the equivalent stiffness of the gas-surface interaction, which subsequently leads to a reduction in the energy accommodation coefficient (EAC) and a suppression of the overall energy exchange [4].

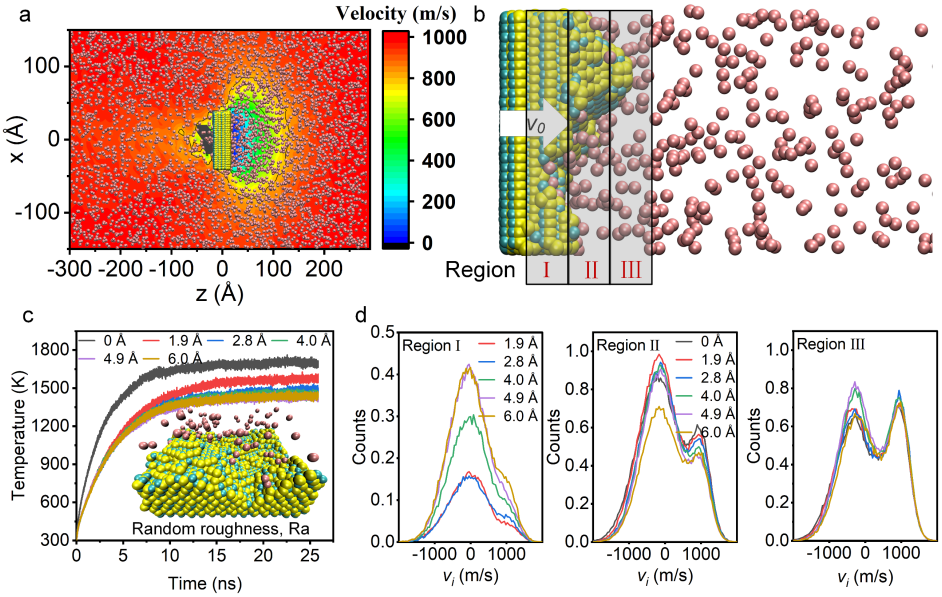


Fig. 1. Thermal shielding effect and velocity distribution of random nano-rough SiC surfaces in high-speed flow.

ACKNOWLEDGEMENTS

This work is supported by the National Natural Science Foundation of China (Grant No. 52505627)

REFERENCES

[1] Q. Han, C. Ma, W. Chen, Z. Wei and Y. Zhang, Applied Surface Science, **657**, 159812 (2024).
[2] Q. Han, H. Xia, W. Chen, G. Wu, J. Li, Z. Wei, F. Zheng and C. Ma, Physics of Fluids, **37 (3)**, 037132 (2025).
[3] P. S. Iyer and K. Mahesh, Journal of Fluid Mechanics, **729**, 524-562 (2013).
[4] J. Sun and Z.-X. Li, Heat transfer engineering, **32 (7-8)**, 658-666 (2011).

Achieving affordable high phase-space resolution for kinetic plasma dynamics via characteristic mapping methods

R.-P. Wilhelm[1,a)], P. Krah[2], F. Bacchini[1,3], K. Kormann[4] and K. Schneider[5]

[1]*Centre for mathematical Plasma Astrophysics, Department of Mathematics, KU Leuven, B-3001 Leuven, Belgium.*
[2]*IRFM - CEA Cadarache, 13108 Saint-Paul-lez-Durance, France.*
[3]*Royal Belgian Institute for Space Aeronomy, Solar-Terrestrial Centre of Excellence, B-1180 Uccle, Belgium.*
[4]*Fakultät für Mathematik, Ruhr-University Bochum, Universitätsstraße 150 D-44780 Bochum*
[5]*Aix-Marseille Université, I2M, CNRS, UMR 7373, 3 place Victor Hugo, 13331 Marseille cedex 3, France.*

[a)]Corresponding author: paul.wilhelm@kuleuven.be

When plasmas are sufficiently rarefied or hot their velocity distributions no longer remain close to equilibrium breaking a crucial assumption of fluid models such as magnetohydrodynamics (MHD). In such cases modeling requires tracking the dynamics of the phase-space distribution functions for each species with the kinetic Vlasov equation coupled to the Maxwell equations for the (self-induced) electro-magnetic fields. Solutions of the Vlasov system are prone to develop fine scale structures due to lack of collisions, while also exhibiting strong multi-scale features due to the differences in mass between the involved electrons and ion-species as well as domain size and dynamic scale. Additionally, the phase-space is up to six-dimensional which in itself already poses a significant numerical challenge.

Particle-In-Cell (PIC) remains the predominant numerical approach to solve the Vlasov equation due to its flexibility in resolving heterogeneous dynamics and geometry, however, suffers from strong noise due to its particle-based nature. [1–3] Hence PIC remains a low-fidelity tool especially if high resolution of the phase-space distribution function is important to correctly capture the dynamics or if low density tails need to be resolved accurately. Grid-based alternatives have by construction close to no noise and therefore are preferred when high-fidelity in phase-space is needed, but they also require relatively high resolutions and careful treatment of the advection to not loose fine-scale structures and conservation properties to numerical diffusion. Hence they are commonly used in combination with simplifying assumptions (such as Gyrokinetics) or in hybrid fluid-kinetic approaches. [4, 5]

Many of the inherent numerical problems of the Vlasov system stem from trying to directly resolve the high-dimensional and complicated phase-space distribution functions. In this talk we will explore the recently proposed alternative *characteristic mapping methods*. [6–10] In contrast to classical Semi-Lagrangian methods, which compute and store the distribution function at every time step, these approaches store the evolution of the characteristics and reconstruct the distribution function from this information when needed. When using the *Numerical Flow Iteration* (NuFI), storage requirements can be reduced further: only the evolution of the smoother electromagnetic fields must be stored, independently of the number of particle species.

Compared to the conceptually related Semi-Lagrangian methods the characteristic mapping approaches such as NuFI with symplectic time-integration preserve all – not only a couple chosen ones – physical invariants such as norms, entropy and total energy, which significantly improves physical fidelity. Additionally, they allow to zoom into regions of interest, without increasing the underlying grid-resolution This allows for high fidelity simulations at low memory cost albeit at somewhat increased computational cost. Finally, there is also some preliminary evidence that through employing the semi-group property of the characteristic map, there is a natural avenue to true low rank compression without destroying underlying structure and while also avoiding prohibitive information loss.

In this talk, we showcase how this paradigm enables high-fidelity simulations of kinetic instabilities and turbulence beyond the reach of classical particle- and grid-based methods, including electron-scale instability dynamics and multi-scale kinetic turbulence test cases.

REFERENCES

[1] J.-L. Vay et al., WarpX: An advanced Particle-In-Cell code, 2018.
[2] F. Bacchini, *The Astrophysical Journal Supplement Series* **268**, 6008 (2023).
[3] S. Fasoulas et al., *Physics of Fluids* **31**, 07200607 (2019).
[4] S. von Alfthan et al., *Journal of Atmospheric and Solar-Terrestrial Physics* **120**, 24–35 (2014).
[5] E. Bourne et al., *J. Open Source Software* **10**, 8582–8582 (2025).
[6] R.-P. Wilhelm et al., *Plasma Physics and Controlled Fusion* **67** (2025).
[7] P. Krah et al., *Communications in Computational Physics* **35**, 905 – 937 (2023).
[8] P. Krah et al., A Hybrid semi-Lagrangian Flow Mapping Approach for Vlasov Systems: Combining Iterative and Compositional Flow Maps, 2026, arXiv:2601.21668 [math.NA] .
[9] R.-P. Wilhelm et al., High fidelity simulations of the multi-species Vlasov-Maxwell system with the Numerical Flow Iteration, 2025, arXiv:2511.23286 [physics.plasm-ph] .
[10] R.-P. Wilhelm et al., Restarting the Numerical Flow Iteration through low rank tensor approximations, 2025, arXiv:2509.08474 [math.NA] .

Efficient Adjoint Optimization of Rarefied Gas Flows

L. Wu[1,a)]

[1]*Southern University of Science and Technology*

[a)]Corresponding author: wul@sustech.edu.cn

Traditional aerodynamic optimization methods have largely been developed for continuum flows, with comparatively little emphasis on rarefied flows, despite their critical importance in applications such as ultra-low Earth orbit vehicles, EUV lithography systems, and vacuum pumping equipment. To address this gap, we develop an adjoint-based shape optimization framework for rarefied gas dynamics that emphasizes computational efficiency. The method employs body-fitted grids and is designed to achieve substantial performance improvements within approximately ten optimization iterations, thereby significantly mitigating the high computational cost associated with rarefied flow simulations. The optimization framework is built upon the General Synthetic Iterative Scheme (GSIS), which provides a deterministic and efficient solution of the Boltzmann model equation. This report presents the fundamental principles of the proposed shape optimization method and demonstrates its preliminary applications to airfoils, jets, and other rarefied-flow systems.

A hybrid kinetic/fluid model based on Kinetic-Diffusion Monte Carlo for neutral particle simulations in plasma edge

Z. Tang[1,a)], T. Steel[1], N. Horsten,[2,3] and G. Samaey[1]

[1]*Department of Computer Science, KU Leuven, Leuven, 3001, Belgium*
[2]*Department of Mechanical Engineering, KU Leuven, Leuven, 3001, Belgium*
[3]*Institute of Mechanics, Materials and Civil Engineering, UCLouvain, Louvain-la-Neuve, 1348, Belgium*

[a)]Corresponding author: zhirui.tang@kuleuven.be

In the plasma edge of nuclear fusion reactors, the neutral transport can be modeled by kinetic equations, and the neutral-related quantities of interest (QoIs) are their macroscopic quantities, i.e., density, velocity, and temperature, corresponding to the first three moments of the solution of the kinetic equation. In reactor-relevant regimes, fully kinetic Monte Carlo (MC) methods, while accurate, become computationally expensive, whereas fluid-limit approximations are fast but may lose accuracy due to boundary effects or low-collisional regimes.

Hybrid kinetic-fluid approaches that combine kinetic and fluid descriptions, therefore, offer a promising alternative. The hybrid methods aim to balance the accuracy of kinetic Monte Carlo approaches and the efficiency of fluid-limit models in the plasma-edge neutral transport simulation. Typical approaches either split the computational domain or decompose the kinetic distribution function into a fluid part and a kinetic part.

In this work, we propose a distribution-decomposition hybrid method for estimating the macroscopic quantities. We start from the kinetic–diffusion Monte Carlo (KDMC) method [1]. KDMC is a asymptotic-preserving hybrid particle method that automatically combines kinetic steps and diffusive steps that represent the accumulated effect of a large number of individual collisions. KDMC behaves as the kinetic MC in low-collisional regimes and converges to the diffusive fluid limit in high-collisional regimes. To apply KDMC to fusion applications, a few issues are addressed.

First, we add the ionization process in KDMC, which so far only included charge exchange collisions.

Second, we propose a QoI estimation scheme. The main issue for neutral QoI estimation using the KDMC particle simulation scheme is that the trajectories do not give information about individual collisions during diffusive steps, rendering classical MC track-length estimation techniques inappropriate. Currently, QoI estimation is done by solving a time-dependent fluid equation, in which the simulation time needs to be approximated [2]. Our scheme, instead, estimates the QoI by solving a steady-state fluid equation, which avoids the simulation-time approximation. More importantly, the proposed estimation framework is expected to be applicable to other hybrid particle simulation methods, in addition to KDMC.

Third, as prior work has shown [3], the accuracy of the QoI estimation depends not only on the quality of KDMC itself, but also on the quality of the fluid model used for estimation. To this end, we introduce a new Navier-Stokes-type fluid model based on a Chapman-Enskog expansion, including the density, momentum, and energy equations. The fluid system leads to much more accurate results than the single fluid equation in [2].

Finally, we implemented outflow and reflective boundary conditions. We propose a parametrized scheme for the reflective boundary condition that interpolates between the kinetic and fluid boundary conditions, and that can be used to balance accuracy with computational speed.

ACKNOWLEDGEMENTS

This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). The views and opinions expressed herein do not necessarily reflect those of the European Commission. The authors are also grateful to Vince Maes and Klaas Willems for valuable discussions.

REFERENCES

[1] B. Mortier, M. Baelmans, G. Samaey, *SIAM Journal on Scientific Computing* **44**, A720–A744 (2022).
[2] B. Mortier, V. Maes, G. Samaey, *Contributions to Plasma Physics* **62** (2022), 10.1002/ctpp.202100197.
[3] Z. Tang, J. Koellermeier, E. Løvbak, G. Samaey, December 2025, 2512.23580 [math] .

Fluid-dynamic limit of the Enskog equation with the guaranteed H-theorem

A. Takahashi[1] and S. Takata[1,a)]

[1] *Department of Aeronautics and Astronautics, Kyoto University, Kyoto-daigaku-katsura, Kyoto 615-8540, Japan*

[a)] Corresponding author: takata.shigeru.4a@kyoto-u.ac.jp

The (original) Enskog equation (OEE) [1] is a pioneering example of a kinetic equation for non-ideal gases, but its H-theorem has not yet been proved. van Beijeren and Ernst proposed the modified (or revised) Enskog equation (MEE) [2] and Resibois established the H-theorem for MEE [3]. However, its complicated structure has hindered its application to numerical studies, so that numerical analyses of dense gases based on kinetic equations have mainly been performed using OEE [4, 5] and its model equations without the H-theorem [6, 7].

The authors recently proposed a new version of the Enskog equation for which the H-theorem is guaranteed [8]. Our modification of the so-called Enskog factor, which is a correction to the collision frequency due to the finite volume fraction, is much simpler than that of MEE, so we refer to our version as the Enskog equation with slight modification (EESM). It was shown that the H-theorem of a form similar to that of MEE holds without taking account of the detailed correlation function between molecular configurations. Because of the simple form of the Enskog factor, EESM requires a computational cost almost equivalent to that of OEE and hence is applicable to numerical simulations.

In the present work, we demonstrate that differences between OEE and EESM in the form of the Enskog factor do not appear on the fluid-dynamic scale by taking its fluid-dynamic limit based on the Chapman-Enskog method [9]. Contrary to the case of equations for ideal gases such as the Boltzmann equation, the small parameters of the asymptotic expansion are not only the Knudsen number but also the dimensionless diameter of molecules. This is because the molecular diameter is proportional to the mean free path and the proportionality constant is of the same order as the volume fraction, which has a finite value for dense gases. Because of this observation, the displacement between centers of two colliding hard-sphere molecules in the Enskog collision operator must be expanded. At leading order, the Euler set of equations with an equation of state (EoS) for non-ideal gases is obtained. OEE and EESM can recover EoS of arbitrary forms including phenomenological EoS such as van der Waals EoS and Carnahan-Starling EoS. A further approximation yields the Navier-Stokes-Fourier set of equations with transport coefficients accounting for non-ideal gas effects. It is shown that, when the same EoS is recovered for both OEE and EESM, their transport coefficients are also perfectly identical to each other. Since it is known that the fluid-dynamic limit of OEE describes the behavior of dense gases well, this result confirms that EESM is consistent with both fluid dynamics and thermodynamics, as is the case for MEE.

ACKNOWLEDGEMENTS

The present work has been supported by the JSPS Grant-in-Aid for JSPS Fellows (No. 24KJ1450).

REFERENCES

[1] D. Enskog, "Kinetic theory of heat conduction, viscosity, and self-diffusion in compressed gases and liquids," in *Kinetic Theory*, Vol. 3, edited by S. G. Brush (Pergamon Press, Oxford, 1972), 226–259.
[2] H. Van Beijeren, M. Ernst, *Physica* **68**, 437–456 (1973).
[3] P. Resibois, *Journal of Statistical Physics* **19**, 593–609 (1978).
[4] A. Frezzotti, *Physics of Fluids* **9**, 1329–1335 (1997).
[5] L. Wu, Y. Zhang, J. M. Reese, *Journal of Computational Physics* **303**, 66–79 (2015).
[6] J. W. Dufty, A. Santos, J. J. Brey, *Physical Review Letters* **77**, 1270–1273 (1996).
[7] B. Shan, W. Su, L. Gibelli, Y. Zhang, *Journal of Fluid Mechanics* **976**, A7 (2023).
[8] S. Takata, A. Takahashi, *Physical Review E* **111**, 065108 (2025).
[9] A. Takahashi, S. Takata, Fluid-dynamic limit of the enskog equation with the guaranteed h-theorem, 2025, arXiv:2507.01341 .

Heat transfer problem of a dense gas described by the Enskog equation with a modification of the Enskog factor

S. Takata[1,a)], **S. Sakata**,[1] and M. Hattori[1]

[1]*Department of Aeronautics and Astronautics, Kyoto University, Kyoto 615-8540, Japan*

[a)]Corresponding author: takata.shigeru.4a@kyoto-u.ac.jp

Recently a study of the dense gas behavior through the kinetic theory attracts attentions, coming from the increasing demands for applications to micro-, submicro-, and even smaller systems. As the system size and the mean free path simultaneously decrease, the molecular size and the volume fraction of molecules become not necessarily negligible, and accordingly the Enskog equation comes into play in place of the Boltzmann equation. Although the Enskog equation with its original form (original Enskog equation, OEE for short) has been successfully applied to fundamental physical problems, thanks to the developments of its numerical methods [1], it does not satisfy the Boltzmann's H theorem, unfortunately. In the meantime, we have recently proposed [2] a variant of the Enskog equation that slightly modifies the Enskog factor in the collision integral (EESM for short), for which the H theorem has been established. This new variant is currently in the early stage of quantitative evaluation for application to physical problems.

In the present work, we revisit the time evolutional heat transfer problem between two parallel plates [3]. On the basis of both OEE and EESM, we numerically observe the time evolution triggered by a sudden temperature change of one plate and evaluate the influence of modifying the Enskog factor.

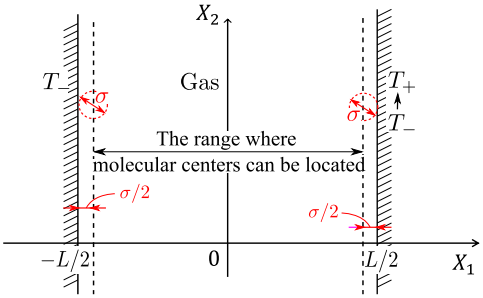


Fig. 1. Problem setting. σ is a diameter of a molecule.

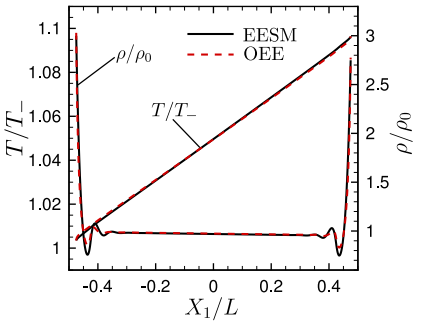


Fig. 2. Comparisons of the profiles of temperature T and density ρ at the steady state for $T_+/T_- = 1.1$, $\sigma/L = 0.05$, and $\eta_0 = 0.25$, where $\eta_0 = (\pi/6)\sigma^3(\rho_0/m)$ with m being the mass of a molecule and ρ_0 is the total mass of the gas divided by $L - \sigma$.

ACKNOWLEDGEMENTS

The present work has been partly supported by the Kyoto University Foundation and by HPCI system Research Project (No. hp250004). A part of computations have been conducted on SQUID at D3 Center, The University of Osaka.

REFERENCES

[1] A. Frezzotti, A particle scheme for the numerical solution of the Enskog equation, *Phys. Fluids* **9**, 1329–1335 (1997); J. M. Montanero and A. Santos, Simulation of the Enskog equation *à la* Bird, *Phys. Fluids* **9**, 2057–2060 (1997); L. Wu, Y. Zhang, and J. M. Reese, Fast spectral solution of the generalized Enskog equation for dense gases, *J. Comput. Phys.* **303**, 66–79 (2015).

[2] S. Takata and A. Takahashi, Enskog and Enskog-Vlasov equations with a modified correlation factor and their H theorem, *Phys. Rev. E* **111**, 065108 (2025).

[3] A. Frezzotti, Monte Carlo simulation of the heat flow in a dense hard sphere gas, *Eur. J. Mech. B/Fluids* **18**, 103–119 (1999); M. Hattori, S. Tanaka, and S. Takata, Heat transfer in a dense gas between two parallel plates, *AIP Advances* **12**, 055220 (2022).

Research on the pumping characteristics of turbomolecular pumps by high-speed incoming gas molecules in the gas capture system of ultra-low orbit aircraft

Kun Sun[1,a)], Mingyang Mao[1], Qiang Liu[1], Jin Qin[1], Chao Yang[2], and Shizhong Zhang[2]

[1] *School of Mechatronics Engineering, Anhui University of Science and Technology, 232001, Huainan, Anhui Province, China.*
[2] *Laboratory for Aerospace Science and Technology, Institute of Mechanics, Chinese Academy of Sciences, 100190, Beijing, China.*

[a)] Corresponding author: ksun@aust.edu.cn

This paper focuses on the research of turbomolecular pumps (TMPs) for gas capture in ultra-low orbit aircraft air-breathing electric propulsion systems. It analyzes the specific performance requirements for TMPs on ultra-low orbit aircraft and points out the design direction for specialized TMPs. Through test particle Monte Carlo methods, the influence of the flight status of incoming gas molecules (i.e., the incident velocity, incident angle, and incident position) on the pumping performance of a single-stage blade TMP is studied, which reveals the pumping mechanism of TMPs for ultra-high-speed gas molecules. Meanwhile, under the background of ultra-high-speed incoming gas molecules, optimization research on the structural parameters of TMP blades is conducted to meet the specific requirements for high pumping speed and lightweight TMPs on ultra-low orbit aircraft. The uniqueness of this paper lies in considering the influence of the flight status of gas molecules after passing through the inlet device on the pumping performance of TMPs. This innovatively combines the inlet device and TMP for research, which can effectively guide the structural design of the inlet device and TMP blades, thereby achieving higher capture efficiency and pressurization effects.

Keywords: Ultra-low orbit aircraft; Gas capture and pressurization; High-speed incoming gas molecules; Turbomolecular pumps; Blade structure optimization

ACKNOWLEDGEMENTS

This work was supported by the National Natural Science Foundation of China [grant number 52305240].

Investigation on the Physics of a rarefied EUV Induced Hydrogen Plasma Jet

W. J. Roog[1,a)] and G. M. W. Kroesen,[1]

[1]*Eindhoven University of Technology, Eindhoven*

[a)]Corresponding author: w.j.roog@tue.nl

Today, the state-of-the-art in microchip manufacturing is Extreme Ultraviolet (EUV) lithography. In a lithography device, the EUV production and EUV lithography stages are spatially separated and operated at different pressures. A small connecting orifice, the intermediate focus, allows EUV radiation to travel between stages. The pressure difference results in a supersonic rarefied jet flow (Kn $\approx$ 0.1), while the intense EUV-radiation partially ionizes H_2. The behavior of EUV-induced plasmas H_2 has been the topic of much recent work [1]. However, the physics of the rarefied EUV induced hydrogen jet remain unexplored. The objective of this work is to characterize and understand the behavior of such a plasma jet. To achieve this, a setup capable of creating a H_2 plasma jet with relevant diagnostics is being developed.

The setup consists of two cylindrical chambers ($r \times h$: 30 $\times$ 60 cm) at high pressure HP and low pressure LP, respectively. The chambers are connected by an interchangeable orifice (initial radius 2.5 mm). H_2 is blown in from the HP side at a controllable rate. The flowrate in combination with the dimensions of the orifice sets the HP side pressure. The LP chamber is pumped by a turbo pump capable of reaching a pumping speed of ~3000 L/s with a correspondingly sized backing pump. The LP side pressure is controlled by adjusting the opening of the turbo pump using a pendulum valve. The operational regime of the setup is characterized by the flowrate, pressure, Mach number, and rarefaction degree. The pressure drop in the setup can be controlled to operate in varying conditions. Based on a 200 Pa -5 Pa pressure drop, the flowrate through the orifice is expected to be ~1.8 SLM H_2 at Mach 1.4. Depending on the exact pressures used, the system will be in the transition between the hydrodynamic and free molecular flow regimes [2].

In the lithography device the plasma is created by photoionization of H_2 by the 92 eV photons. In contrast, the initial plasma in the setup is generated using a collisional microwave source (SAIREM Hi-Wave) [3]. The source consists of a generator capable of supplying up to 450 W in 2.45 GHz microwaves and an alumina antenna in the HP-chamber. The injected microwaves accelerate free electrons to energies higher than the H_2 ionization threshold, igniting the plasma. In H_2 the Hi-wave is capable of maintaining electron densities in the range of 10^{17} m^{-3}. The plasma is generated 5 cm behind the orifice and is dragged along with the supersonic flow. This creates the desired H_2 plasma jet. We will report on initial measurements focused on the flow aspect of the jet.

ACKNOWLEDGEMENTS

This research has been sponsored in part by Holland High Tech and by ASML.

REFERENCES

[1] J. Beckers, T. Van De Ven, R. Van Der Horst, D. Astakhov, V. Banine, *Applied Sciences* **9**, 2827 (2019).
[2] F. Sharipov, *Journal of Fluid Mechanics* **518**, 35–60 (2004).
[3] L. Latrasse, M. Radoiu, T. Nelis, O. Antonin, *Journal of Microwave Power and Electromagnetic Energy* **51**, 237–258 (2017).

Frequency-domain general synthetic iterative scheme for efficient simulation of oscillatory rarefied gas flows

Pengshuo Li[1] and Lei Wu[1,a)]

[1]*Department of Mechanics and Aerospace Engineering, Southern University of Science and Technology, Shenzhen 518055, China.*

[a)]Corresponding author: wul@sustech.edu.cn

Oscillatory rarefied gas flows are frequently encountered in micro-electro-mechanical systems, and their efficient numerical simulation remains a major challenge due to the time-dependent nature of the problem and the high dimensionality of the Boltzmann kinetic equation [1]. Here, we address this challenge by focusing on the periodic steady state and solving the resulting problem using the frequency-domain general synthetic iterative scheme (GSIS) [2]. The core idea is to couple the mesoscopic kinetic equation with macroscopic synthetic equations: the kinetic equation supplies higher-order constitutive information beyond Newton's viscosity and Fourier's heat conduction laws, while the synthetic equations converge to the periodic steady state much faster and thus accelerate the kinetic iteration. As a result, super convergence is achieved, together with an asymptotic-preserving property that allows the use of coarse spatial grids. The resulting frequency-domain GSIS can be up to three orders of magnitude faster than conventional kinetic schemes in near-continuum regimes. The method is applicable to representative oscillatory rarefied flows (e.g., shear-driven oscillatory flows and squeeze-film damping), offering an efficient and robust frequency-domain kinetic framework for MEMS gas damping simulations.

REFERENCES

[1] L. Wu, J. M. Reese, Y. Zhang, *Journal of Fluid Mechanics* **748**, 350–367 (2014).
[2] W. Su, L. Zhu, P. Wang, Y. Zhang, L. Wu, *Journal of Computational Physics* **407**, 109245 (2020).

Machine-learning-based derivation of moment closures for strongly nonequilibrium flows

H. Song[1,a)], S. Singh[1] and M. Torrilhon[1]

[1]*RWTH Aachen, Germany*

[a)]Corresponding author: hang.song@rwth-aachen.de

Gas flows under rarefied and hypersonic conditions frequently depart far from thermodynamic equilibrium, posing fundamental difficulties for continuum-based descriptions. These difficulties mainly arise from the inability of conventional Navier-Stokes Fourier formulations to represent pronounced nonlinearity in transport processes and the influence of higher-order velocity moments. In this study, a hybrid modeling strategy is introduced in which machine learning is employed to augment the regularized 13-moment (R13) equations.

The proposed approach replaces selected analytical closures in the R13 system with data-driven representations. Fully connected neural networks are constructed using datasets generated by direct simulation Monte Carlo (DSMC) calculations, enabling the learning of nonlinear relationships associated with higher-order moments and collisional production terms. The training data are extracted from one-dimensional stationary shock-wave configurations, and a dedicated methodology is developed to recover collision integrals directly from DSMC statistics.

Once trained, the neural-network-based closures are embedded within a discontinuous Galerkin spectral element solver, yielding a computational framework that retains the conservation properties and structural consistency of the original R13 equations. Validation against DSMC benchmarks shows that the resulting model captures shock thickness, stress components, heat fluxes, and several higher-order moments with significantly improved fidelity over a broad range of Mach numbers, including regimes not represented in the training data.

Further numerical investigations demonstrate that the framework remains effective for unsteady flow scenarios dominated by strong nonequilibrium dynamics. When compared with both the conventional R13 formulation and the Navier2̌013Stokes2̌013Fourier equations, the present hybrid model delivers enhanced stability and predictive accuracy. Overall, this work demonstrates that machine-learning-based constitutive closures offer a promising pathway for extending continuum models of rarefied gas flows, achieving substantially improved accuracy while maintaining computational efficiency well below that of fully kinetic simulations, and thereby supporting practical hypersonic aerothermodynamic analyses.

Surrogate-assisted airfoil optimization in rarefied gas flows

X. Li[1,a)], R. Yuan[1], Y. Zhang[1] and L. Wu[1]

[1]*Department of Mechanics and Aerospace Engineering, SUSTech, Shenzhen, 518055, China*

[a)]Corresponding author: wul@sustech.edu.cn

With growing interest in space exploration, optimized airfoil design has become increasingly important. However, airfoil design in rarefied gas flows remains underexplored because solving the Boltzmann equation formulated in a six-dimensional phase space is time-consuming. To address this problem, a solver-in-the-loop Bayesian optimization framework for symmetric, thickness-only airfoils is developed. First, airfoils are parameterized using a class shape transformation that enforce geometric admissibility. Second, a Gaussian-process expected-improvement surrogate is coupled in batches to a fast-converging, asymptotic-preserving Boltzmann solver for sample-efficient exploration. Drag-minimizing airfoils are identified in a wide range of gas rarefaction. It is found that, at Mach numbers $M_\infty = 2$ and 4, the dimensionless streamwise drag increases with the gas rarefaction and shifts from pressure-dominated to shear-dominated, while optimization reduces drag at all conditions. The benefit of optimization peaks in the weakly rarefied regime — about 30 percent at $M_\infty = 2$ and 40 to 50 percent at $M_\infty = 4$ — and falls to a few percent in transition and free-molecular flow regimes. Drag decomposition shows that these gains come mainly from reduced pressure drag, with viscous drag almost unchanged. The optimal airfoils form a coherent rarefaction-aware family: they retain a smooth, single-peaked thickness profile, are aft-loaded at low gas rarefaction, and exhibit a forward shift of maximum thickness and thickness area toward mid-chord as gas rarefaction increases. These trends provide a physically interpretable map that narrows the design space and offers practical guidance for rarefied aerodynamic shaping.

Laser Absorption Measurements of Nitric Oxide Formation in Air with High Vibrational State Resolution

J. W. Streicher,[a)] Devin P. Merrell, Dylan L. Drescher, and R. K. Hanson

Department of Mechanical Engineering Stanford University 440 Escondido Mall Stanford California 94305 USA

New ring-amplified shock tube (RAST) methods have enabled the extended application of tunable diode laser absorption spectroscopy (TDLAS) for probing species and states with low populations by substantially extending the effective absorbing pathlength in reflected shock studies. This new technique has now been applied to a variety of species and states, ranging in application from fundamental spectroscopy, ammonia combustion, vibrational energy excitation, and plasma formation [1, 2, 3, 4]. Now, similar methods have been extended to probe nitric oxide formation in air and air/argon mixtures. Initial diagnostic development was pursued for a 6% O_2, 6% N_2, 88% Ar mixtures, which demonstrated the ability to resolve the ground to fourteenth excited vibrational states of NO (v" = 0-14) [5]. However, the utility of this strategy has been extended through application to air (21% O_2 in N_2) and air diluted in equal parts with argon (50% air, 50% Ar). These mixtures provide ample opportunities to investigate NO formation through the Zeldovich reactions, while the Ar dilution extends test time such that subsequent NO dissociation reactions can be observed. Results from these reflected shock experiments, with post-shock initial conditions ranging from 3640 - 7570 K and 0.06 - 0.90 atm, show the low scatter and uncertainty available via the sensitive RAST methods (Fig. 1).

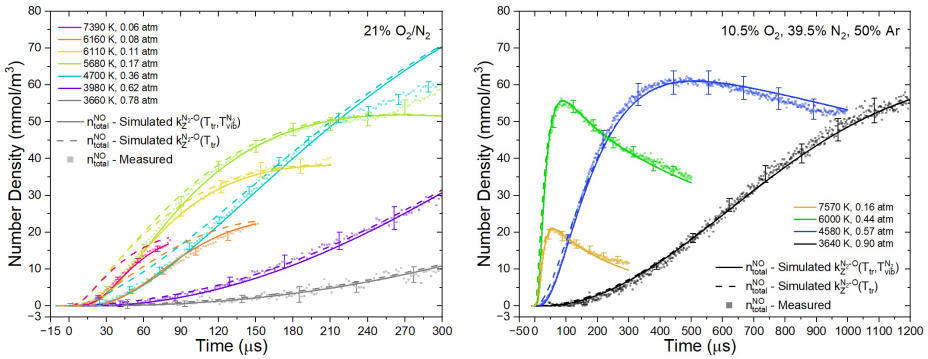


Fig. 1. Measured NO number density time-histories in air (left) and air diluted equally with argon (right). Notably, argon dilution substantially extends the experimental test time, allowing observation of a peak in NO formation followed by subsequent dissociation reactions. A best-fit model – with updated Zeldovich and NO dissociation reaction rates – is provided to demonstrate the observed delay in NO formation between a single temperature Zeldovich rate (dashed) and the two-temperature (T_{tr} and $T_{vib}^{N_2}$) best fit rate (solid).

Although this abstract only provides the total NO number density profiles (n_{total}^{NO}), the TDLAS data, which includes absorption profiles from v" = 0-14, has been further analyzed to investigate modal temperatures and vibrational-state-specific population time-histories. Modal temperatures – both rotational (T_{rot}^{NO}) and vibrational (T_{vib}^{NO}) – are resolved with very low scatter and uncertainty due to the wide range of overlapping rovibrational content in the 1580 - 1589 cm^{-1} region of the quantum cascade laser. These modal temperatures both complement prior measurements made with UV laser diagnostics as well as aid inferences of reaction rates throughout the temperature evolution present during each experiment. Furthermore, vibrational-state-specific population time-histories enable the evaluation of Boltzmann distributions of vibrational states. Ultimately, these new vibrational-states-specific NO measurements will substantially improve rate inferences and enable subsequent model evaluation and refinement for high-temperature air.

REFERENCES

[1]C. L. Strand, D. Merrell, A. Thoeny, J. W. Streicher, and R. K. Hanson, "Ring-amplified shock tube for variable-gain, multi-wavelength absorption spectroscopy," Opt. Express **33**, 42653–42676 (2025).

[2]T. M. Rault, P. P. Simha, J. W. Streicher, C. L. Strand, and R. K. Hanson, "A shock tube and pathlength-amplified laser absorption study of hydrazine pyrolysis," in *14th US National Combustion Meeting* (2025).

[3]D. Merrell, A. Thoeny, C. L. Strand, and R. Hanson, "High temperature collisional broadening of the oxygen A-band for partners O_2, N_2, and Ar," Journal of Quantitative Spectroscopy and Radiative Transfer **348**, 109683 (2026).

[4]D. P. Merrell, D. L. Drescher, Z. N. Granowitz, J. W. Streicher, C. Strand, and R. K. Hanson, "Pathlength-amplified tunable diode laser absorption spectroscopy of the excitation and ionization of air in a shock tube," in *AIAA SCITECH Forum* (2026).

[5]J. W. Streicher, D. P. Merrell, D. L. Drescher, C. Strand, and R. K. Hanson, "Vibrational-state-resolved measurements of nitric oxide for the ground to fourteenth excited vibrational state," in *AIAA SCITECH Forum* (2026).

[a)]Corresponding author: jessewst@stanford.edu

Abstract 50

Failure of NS Equation in Jet Turbulence

S. Tian[1], L. Wu[1,a)]

[1] *Department of Mechanical and Aerospace Engineering, Southern University of Science and Technology, Shenzhen, China.*

[a)] Corresponding author: wul@sustech.edu.cn

Turbulent flows in near-vacuum environments challenge the validity of the classical Navier–Stokes (NS) equations, particularly when rarefaction and unsteadiness coexist. In this work, a dual turbulent jet impingement configuration representative of the near-vacuum lunar landing conditions is used to examine the physical mechanisms underlying NS equation failure in rarefied turbulence. The Knudsen number and Reynolds number of the Mach 5.45 jets based on nozzle diameter are 0.000687 and 11800, respectively.

Direct transient simulations based on the Boltzmann equation are performed alongside corresponding NS-based simulations, enabling a time-resolved comparison of unsteady flow evolution, stress transport, and surface loading. The results show that, despite moderate global rarefaction levels, the NS equations fail to capture key unsteady features of the flow, including shock–shear interactions and wall heat flux distributions.

More importantly, the observed breakdown is not caused by large non-equilibrium stresses themselves, but by a local degeneracy of the leading-order continuum description. Under specific kinematic conditions, the Newtonian shear stress collapses, allowing formally higher-order non-equilibrium corrections to dominate the local stress balance and be dynamically amplified.

These findings reveal a distinct physical route to NS equation failure in turbulent rarefied flows and highlight the necessity of non-equilibrium modeling for jet–surface interaction problems.

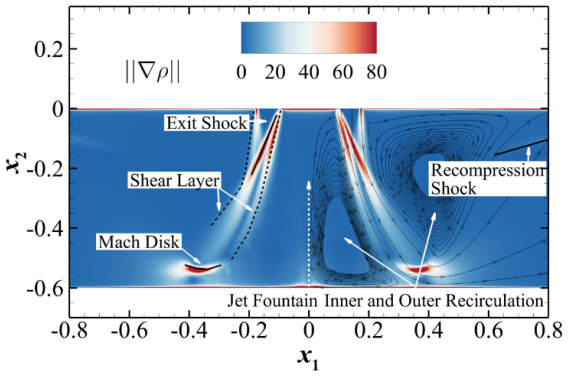


Fig. 1. Density gradient magnitude of the jet impingement flow field, with key structures noted.

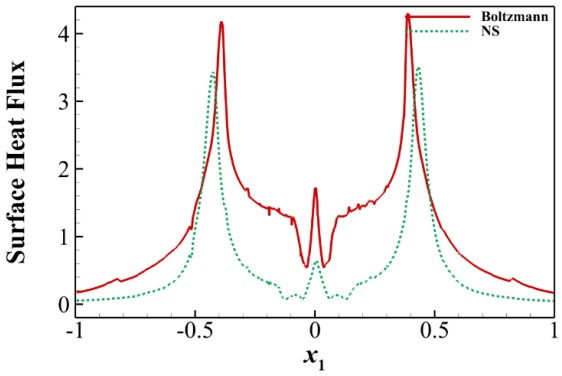


Fig. 2. Ground heat flux distributions from the Boltzmann and the NS simulations.

ACKNOWLEDGEMENTS

This work was supported by the National Natural Science Foundation of China (Grant No.~12450002)

REFERENCES

[1] S. Tian, L. Wu. Small Rarefaction, Large Consequences: Limits of Navier Stokes Turbulence Simulations. *arXiv preprint arXiv*:2602.08770 (2026).

Abstract 51

Discrete Rotational Energy for Polyatomic Molecules in Direct Simulation Monte Carlo

D. S. Liechty[1,a)], D. Crouse[2], and T. E. Schwartzentruber[2]

[1] *NASA Langley Research Center, Aerothermodynamics Branch, Hampton, VA 23681.*
[2] *University of Minnesota, Minneapolis, MN 55455.*

[a)] Corresponding author: Derek.S.Liechty@nasa.gov

The environments experienced by vehicles upon entry into planetary atmospheres generally result in severe aerothermodynamic loading. These flows are characterized by the formation of strong shock waves, behind which high temperatures and non-equilibrium environments are generated, and the accurate prediction of internal energy relaxation and chemical kinetics becomes important. This manuscript focuses on the internal relaxation of the rotational energy of polyatomic molecules. Previous work [1] has described the implementation of a discrete rotational energy model for diatomic molecules (linear rotators). Later, Gimelshein et. Al [2] extended this model to include polyatomic molecular internal energies. However, they did not include details on how to generate the particles at equilibrium conditions and centrifugal distortion was not included in their model.

The purpose of the present study is to extend the afore-mentioned models to the treatment of discrete rotational energy in polyatomic molecules with the addition of centrifugal distortion. An overview of the background theory needed for the implementation of the model will be given followed by the model itself and verification of the model. For example, sampled versus Boltzmann distributions are compared in Figure 1 for CH_3 (oblate rotator – two quantum numbers) and examples of thermal relaxation behavior for linear and non-linear rotators are presented in Figure 2. In addition, comparisons of thermophysical properties will be presented, as well as examples of adiabatic relaxation and application to hypersonic flow.

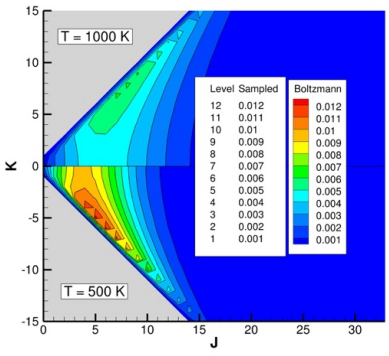


Fig. 1. Rotational level distribution for CH_3.

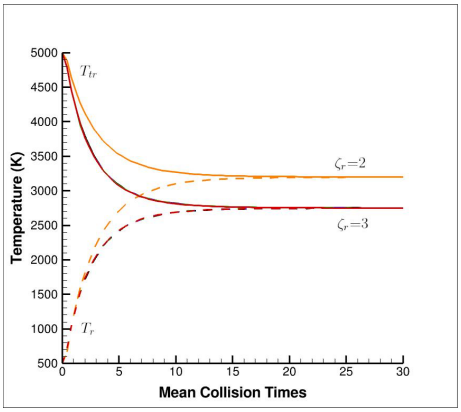


Fig. 2. Thermal relaxation of an adiabatic reactor to equilibrium for rotational excitation.

ACKNOWLEDGEMENTS

The authors would like to thank the Minnesota Space Grant Consortium (MnSGC) [Grant Number 80NSSC20M0111] for internship funding.

REFERENCES

[1] I. D. Boyd, *Physics of Fluids A,* **5**, pp. 2278-2286 (1993).
[2] S.F. Gimelshein, et al., AIAA Paper 99-0738 (1999).

Lattice Boltzmann schemes for parabolic problems under monotonicity conditions

D. Aregba[1,a)], N. Bonamy Parrilla[1] and S. Brull[1]

[1] *Institut de mathématiques de Bordeaux*

[a)] Corresponding author: Stephane.Brull@math.u-bordeaux.fr

Many applications require solving parabolic equations such as drift equations for cold plasmas. In this talk we investigate Lattice Boltzmann Scheme inspired from Aregba-Natalini-Tang approach ([1]) for nonlinear parabolic systems in the case of discrete BGK schemes. Our objective is to extend existing results to a broader class of parabolic problems and to assess the robustness of theses schemes in practical situations under monotonicity conditions.

References

[1] Aregba-Driollet, D.; Natalini, R.; Tang, S., Explicit diffusive kinetic schemes for nonlinear degenerate parabolic systems, Math. Comp. 73 (2004), no. 245, 63$\tilde{2}$01394

Rovibronic Energy Transfer and Reactive Processes in Direct Simulation Monte Carlo

Clément H. B. Civrais[1,a] and Marcel Pfeiffer[2]

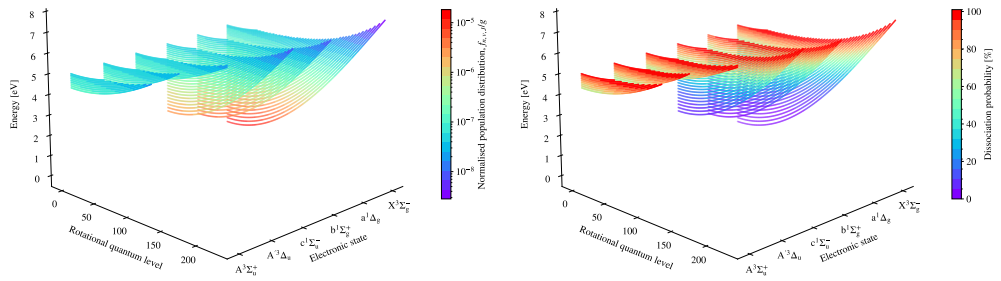
[1]*Department of Mechanical and Aerospace Engineering, University of California, Irvine, CA 92697, USA.*
[2]*Institute of Space Systems, University of Stuttgart, Pfaffenwaldring 29, 70569 Stuttgart, Germany.*

[a]Corresponding author: ccivrais@uci.edu

In the past two decades, the quasi-classical trajectory (QCT) method using first principle potential energy surfaces (PES) has become a standard for gaining physical insights into collisional systems, e.g. O_2 + O and O_2 + O_2. To date, most of the QCT calculations for collisional systems relevant to hypersonic applications are conducted on adiabatic potential energy surfaces. Indeed, the O_2 + O and O_2 + O_2 collisional systems were described with a global potential energy surface involving 12 states that govern electronically adiabatic collisions of ground-electronic state collisions [1, 2]. However, there exist six electronic states of O_2 lying below the dissociation energy which may likely contribute to the kinetic processes. Specifically, past studies have demonstrated that for these high-fidelity calculations to accurately recover experimental measurements [3, 4], the dissociation rate coefficients must be scaled by a multi-surface factor that correlates to the degeneracy of the electronic excited states.

To resolve this limitation, one must perform QCT calculations on diabatic potential energy surfaces. In the past five years, progress has been made by the theoretical chemistry community to develop a series of diabatic PES for the O_2 + O collisional systems involving the dynamics of the electronic excited states [5]. However, these PESs were developed for a single spin state, preventing full characterisation of the contribution of the electronic excited states. To date, no state-to-state kinetic database has yet been constructed on the O_2 + O collisional system, allowing to gain of insights into the contribution of the electronic excited states for the dissociation of oxygen.

The present article addresses such limitations by constructing a kinetic database by leveraging the quantum kinetic (QK) chemistry model [6] developed for the direct simulation Monte Carlo (DSMC) [7]. The present article proposes a kinetic scheme for the dissociation of molecular oxygen that accounts for the contributions of electronic excited states. An example of the predictions of the model for the population internal degrees of freedom of O_2 and dissociation probability is depicted in Fig. 1. The predictions of the kinetic scheme are assessed for a compilation of experimental measurements [3, 4] and high-fidelity chemistry calculations [1, 2] in both thermal equilibrium and non-equilibrium conditions. Then, the kinetic scheme is validated against shock tube experiments of Ibraguimova *et al.* [3]. Finally, a master equation analysis is conducted to gain physical insights into the contribution of the electronic excited states in post-shock and expanding flow conditions.



(a) Normalised distribution function **(b)** Dissociation probability

Fig. 1. Rovibronic state-specific population distribution and dissociation probability of O_2 at T = 10,000 K.

REFERENCES

[1] M. S. Grover, E. Torres, T. E. Schwartzentruber, *Physics of Fluids* **31**, 076107 (2019).
[2] S. M. Jo, S. Venturi, J. G. Kim, M. Panesi, *The Journal of Chemical Physics* **158**, 064305 (2023).
[3] L. B. Ibraguimova, A. L. Sergievskaya, V. Y. Levashov, O. P. Shatalov, Y. V. Tunik, I. E. Zabelinskii, *The Journal of Chemical Physics* **139**, 034317 (2013).
[4] J. W. Streicher, A. Krish, R. K. Hanson, *Physics of Fluids* **33**, 056107 (2021).
[5] Y. Shu, F. B. Akher, H. Guo, D. G. Truhlar, *The Journal of Physical Chemistry A* **128**, 1207–1217 (2024).
[6] G. A. Bird, *Physics of Fluids* **23**, 106101 (2011).
[7] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Oxford University Press Inc, 1994).

Abstract 55

Topology of machine-learned DSMC constitutive relations in rarefied Couette flow and the proof of the elliptic constraint

G. Garg[1], T. K. Mankodi[2], and R. S. Myong[1,a)]

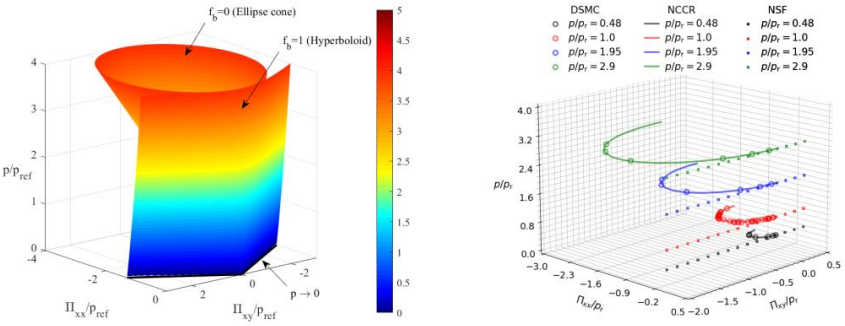
[1] *School of Mechanical and Aerospace Engineering and ACTRC, Gyeongsang National University, Jinju, Gyeongnam 52828, South Korea*

[2] *Department of Mechanical Engineering, Indian Institute of Technology Guwahati, Guwahati, Assam 781039, India*

[a)] Corresponding author: myong@gnu.ac.kr

While constitutive relations (CRs) are fundamental to rarefied gas dynamics, they exhibit pronounced nonlinearity in non-equilibrium regimes, where the conventional Navier–Stokes–Fourier (NSF) laws break down. This study uses a pressure-consistent direct simulation Monte Carlo (DSMC) [1] database for planar Couette-type flows spanning a wide range of Knudsen and Mach numbers to characterize three flow structures: (i) the topology of the elliptic stress constraint, (ii) the topology of the heat-flux constraint, and (iii) the organization of the CR map, in the DSMC solution space. For the normalized viscous stress pair, nonlinear coupled constitutive relations (NCCR) predict a quadratic constraint: at fixed normalized pressure, the constraint is an ellipse, and when the pressure varies, it forms a cone [2, 3]. Figure 1 visualizes the elliptic stress constraint predicted by NCCR theory and its point-by-point validation against the DSMC solution.

Furthermore, motivated by prior machine-learned DSMC-CR developments [4, 5], the present work extends the framework to velocity-shear flows. These DNN-based CRs are embedded in a finite-volume solver with consistent wall slip/jump treatments [2], enabling DSMC-level predictions of conserved and non-conserved quantities under untrained conditions with computational cost close to NSF simulations.



(a) Conic topology of the NCCR theory (Reproduced from Singh *et al.* [3])

(b) Comparison of topologies for DSMC, NCCR, and NSF (monatomic gas)

Fig. 1. The topology of the stress constraint for velocity-shear flows: NCCR and DSMC.

ACKNOWLEDGEMENTS

This work was supported by the US AFOSR Grant No. FA2386-22-1-4051. The authors also acknowledge partial support provided by the KASA (RS-2022-NR067079) and NRF (RS-2024-00397400), Republic of Korea.

REFERENCES

[1] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Oxford University Press, 1994).
[2] R. S. Myong, *Physics of Fluids,* **28(1)**, 012002 (2016).
[3] S. Singh, A. Karchani, K. Sharma, R. S. Myong, *Physics of Fluids,* **32(2)**, 026104 (2020).
[4] G. Garg, T. K. Mankodi, E. Esmaeilifar, R. S. Myong, *Physics of Fluids,* **36(10)**, 106113 (2024).
[5] G. Garg, T. K. Mankodi, R. S. Myong, *Physics of Fluids,* **37(7)**, 076105 (2025).

Abstract 56

A finite-volume solver with machine-learned constitutive relations for non-equilibrium flows under strong compression and expansion

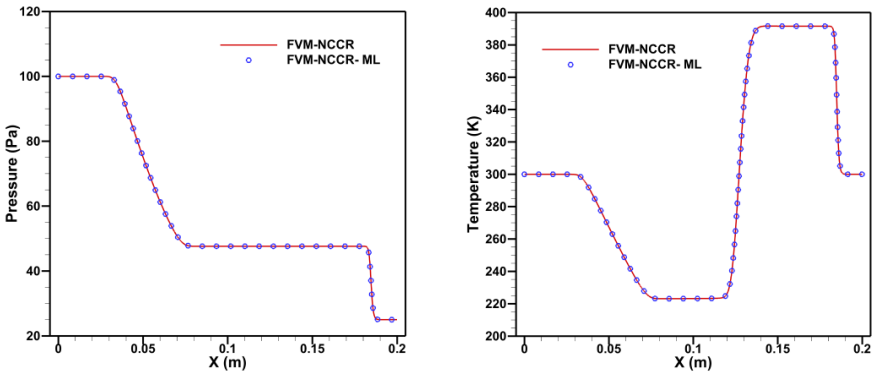
G. Garg[1], T. K. Mankodi[2], and R. S. Myong[1,a)]

[1] *School of Mechanical and Aerospace Engineering and ACTRC, Gyeongsang National University, Jinju, Gyeongnam 52828, South Korea*
[2] *Department of Mechanical Engineering, Indian Institute of Technology Guwahati, Guwahati, Assam 781039, India*

[a)] Corresponding author: myong@gnu.ac.kr

Unsteady rarefied gas dynamics often require direct simulation Monte Carlo (DSMC) [1] to capture non-equilibrium transport, but DSMC becomes costly for multi-wave transients. Building on Myong's [2] idea that a database of non-equilibrium constitutive relations can augment a finite-volume (FV) solver with near-NSF cost, Garg et al. [3, 4] developed a machine-learned (ML) closure trained in the compression regime and demonstrated DSMC-level accuracy for one-dimensional steady shock structures.

Here, we extend constitutive learning to non-equilibrium flows under strong compression and expansion by developing ML constitutive models valid for both the shock (compression) and rarefaction (expansion) branches. The closure is trained to reproduce non-equilibrium constitutive behavior using two complementary sources: (i) a nonlinear coupled constitutive relation (NCCR) formulation (second-order in nature) and (ii) DSMC-derived constitutive relations. The resulting FV solver equipped with the ML constitutive closure is validated on the transient Sod shock-tube problem, which contains both a shock and a rarefaction fan. Comparisons focus on time-resolved macroscopic fields and non-equilibrium fluxes (viscous stress and heat flux). A representative FV–NCCR–ML validation for a Sod case is shown in Fig. 1.



(a) Pressure (b) Temperature

Fig. 1. Sod shock-tube comparison of the FVM–NCCR–ML solver with the FVM–NCCR solver: pressure and temperature profiles at a time ($t = 2.0 \times 10^{-4}$ s).

ACKNOWLEDGEMENTS

This work was supported by the US AFOSR Grant No. FA2386-22-1-4051.

REFERENCES

[1] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Oxford University Press, 1994).
[2] R. S. Myong, *Physics of Fluids*, **11(9)**, 2788-2802 (1999).
[3] G. Garg, T. K. Mankodi, E. Esmaeilifar, R. S. Myong, *Physics of Fluids*, **36(10)**, 106113 (2024).
[4] G. Garg, T. K. Mankodi, R. S. Myong, *Physics of Fluids*, **37(7)**, 076105 (2025).

KitAMR.jl: An Adaptive Mesh Based, Efficient and Scalable DVM Solver

L. Ge[1,a)], T. Xiao[2,3] and Q. Cai[1]

[1]*Department of Mechanics, School of Mechanics and Engineering Science, Peking University, Beijing, China*
[2]*Centre for Interdisciplinary Research in Fluids, Institute of Mechanics, Chinese Academy of Sciences, Beijing China*
[3]*School of Engineering Science, University of Chinese Academy of Sciences, Beijing, China*

[a)]Corresponding author: gelq@stu.pku.edu.cn

The transition flow regime is crucial to rarefied gas dynamics. The Discrete Velocity Method (DVM) captures non-equilibrium physics through the evolution of discrete distribution functions[1], enabling the solution of flows with any Knudsen number. Despite advantages over direct simulation methods in transition flows, the increase in dimensions still results in high computational costs for DVM. Meanwhile, rarefied gas flows often involve discontinuities, and under extreme flight conditions, the distribution function can exhibit both highly concentrated and widely dispersed characteristics[2]. The scenarios place high demands on the resolution in physical and velocity space. Large multi-scale computations of DVM is a research area worth exploring[3], yet there is no efficient, open-source programs currently available in the field.

Adaptive Mesh Refinement (AMR) reallocates computational resources based on flow features, balancing efficiency and accuracy[4]. The ongoing project discretizes with tree-based Cartesian grids, adapting the mesh in both physical and velocity space according to characteristics including velocity field gradients, boundary complexity, and energy proportion at phase points. By employing a specially designed Immersed Boundary Method (IBM), the proposed distributed DVM solver maintains accuracy at boundaries and enhances universality[5], suited for multi-scale complex flows across a wide range of regimes.

Additionally, schemes are typically built on model equations that inevitably introduce phenomenological artificial parameters[6], leaving room for model-level optimization. Automatic differentiation advantages the solver in areas like machine learning, supporting model optimization.

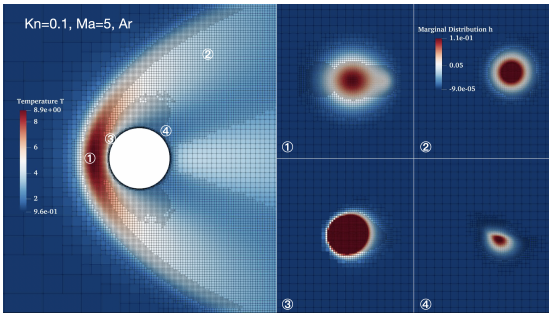


Fig. 1. A hypersonic flow over a cylinder. The adaptation mesh refinements(AMR) in physical space(left) and velocity space(right) are simultaneously applied. The cylinder is resolved by the Immersed Boundary Method(IBM)[5].

ACKNOWLEDGEMENTS

The current research is funded by Strategic Priority Research Program of Chinese Academy of Sciences (XDB0620403), Chinese Academy of Sciences Project for Young Scientists in Basic Research (YSBR107), National Science Foundation of China (12302381, 12572340), and Beijing Natural Science Foundation (L252039). The computing resources provided by Hefei Advanced Computing Center are acknowledged

REFERENCES

[1] K. Xu, J.-C. Huang, *Journal of Computational Physics* **229**, 7747–7764 (2010).
[2] S. Chen, K. Xu, C. Lee, Q. Cai, *Journal of Computational Physics* **231**, 6643–6664 (2012).
[3] Y. Zhu, K. Xu, *arXiv preprint arXiv:2102.01261* (2021).
[4] Z. Wang, *Computers & Fluids* **27**, 529–549 (1998).
[5] L. Ge, Q. Cai, Y. Zhang, T. Xiao, *arXiv preprint arXiv:2512.20252* (2025).
[6] P. L. Bhatnagar, E. P. Gross, M. Krook, *Physical review* **94**, 511 (1954).

Non-equilibrium simulations of monatomic rarefied gas flows based on Grad's 20-moment equations

Satyvir Singh[a)] and Manuel Torrilhon

Institute for Applied and Computational Mathematics, RWTH Aachen University, Germany

[a)]Corresponding author: singh@acom.rwth-aachen.de

Non-equilibrium gas flows in the rarefied–continuum transition regime arise in many applications involving high-speed aerodynamics, microscale gas transport, and shock-driven compressible flows [1]. In such regimes, the classical Navier–Stokes–Fourier equations fail to accurately represent transport processes due to strong thermodynamic non-equilibrium and finite-Knudsen-number effects [2]. Kinetic approaches such as the Boltzmann equation provide accurate descriptions but remain computationally expensive for multidimensional problems. Moment-based models derived from kinetic theory therefore offer an attractive intermediate description that bridges continuum and kinetic formulations [3]. In this work, non-equilibrium flow simulations of monatomic rarefied gases are performed using Grad's 20-moment equations, which extend classical hydrodynamic models by incorporating higher-order stress and heat-flux transport effects. Compared with lower-order moment systems, the Grad-20 formulation improves the representation of non-equilibrium transport phenomena and shock-layer structures in moderate-Knudsen-number flows.

A high-order discontinuous Galerkin (DG) method is employed for the spatial discretization of the governing moment system. The DG framework provides high-order accuracy, geometric flexibility, and improved stability for convection-dominated problems with discontinuities [4, 5]. Numerical fluxes and time integration strategies are designed to maintain stability in the presence of strong gradients and shock waves. The proposed numerical framework is validated using several canonical compressible-flow problems exhibiting strong non-equilibrium behavior. These include the Sod shock tube problem, steady normal shock-wave structure, shock–vortex interaction, and shock–bubble interaction. These test cases involve discontinuities, multi-scale wave interactions, and localized non-equilibrium regions, making them suitable benchmarks for higher-order moment models. Simulation results demonstrate that the Grad-20 moment system captures non-equilibrium transport effects that are not represented in classical continuum models while remaining significantly more efficient than kinetic solvers. In summary, the present study demonstrates that Grad-20 moment equations combined with high-order DG discretization provide a robust and computationally efficient framework for simulating shock-dominated non-equilibrium rarefied gas flows [6].

ACKNOWLEDGEMENTS

The authors acknowledge funding through the German Research Foundation within the research unit DFG–FOR5409.

REFERENCES

[1] H. Struchtrup, *Macroscopic Transport Equations for Rarefied Gas Flows* (Springer, 2005).
[2] M. Torrilhon, *Annual Review of Fluid Mechanics* **48**, 429–458 (2016).
[3] H. Grad, *Communications on Pure and Applied Mathematics* **2**, 331–407 (1949).
[4] B. Cockburn, C.-W. Shu, *Journal of Scientific Computing* **16**, 173–261 (2001).
[5] S. Singh, A. Karchani, T. Chourushi, R. S. Myong, *Journal of Computational Physics* **457**, 111052 (2022).
[6] M. Torrilhon, *Multiscale Modeling & Simulation* **5**, 695–728 (2006).

Implementation of Surface Radiation to SPARTA's Hypersonic Ablation Model

F. Ramin[1,a)], L. Bott,[1] and **C. Stemmer**[1]

[1]*Chair of Aerodynamics and Fluid Mechanics, Technical University of Munich, 85748 Garching b. München, Germany*

[a)]Corresponding author: Falk.ramin@tum.de

Thermal Protection Systems (TPSs) are essential for safe atmospheric re-entry. For high-energy returns (e.g., lunar trajectories), non-reusable ablative shields are typically used, yet their designs remain conservative due to modeling uncertainty. While peak heating occurs at lower altitudes where continuum CFD is applicable, ablation begins at higher altitudes in the rarefied regime, where Direct Simulation Monte Carlo (DSMC) methods are required. Stochastic PArallel Rarefied-gas Time-accurate Analyzer (SPARTA) is an open-source DSMC code, able to simulate ablation in these regions. In previous work, Bott [1] and Chen *et al.* [2] implemented a new ablation rule in the open-source DSMC code SPARTA, which couples the material response with the free-stream using the integral heat balance on the geometry-surface to simulate ablation and surface recession on a macroscopic, capsule-size scale. Thereby, the ablation is determined by the particles' kinetic energy, decoupling the surface recession from the mesh size and the number of nodes. However, in this ablation model, no local varying surface temperature is implemented for implicit meshes. Therefore, the surface radiation is omitted in the heat balance equation, resulting in significantly larger recession rates than those observed in experiments.

This study continues and expands the work by Bott [1] introducing a locally varying, time-dependent surface temperature for implicit meshes and implementing an improved surface energy balance in SPARTA's ablation model that includes the radiative heat loss. The diffuse reflection model in SPARTA is modified to determine the post-collision particle properties based on the newly implemented local surface temperature. The computation of the convective particle flux onto the ablation surface has been improved, now using the kinetic-energy difference between pre- and post-collision velocities instead of the prior rule used in [1], which considered only the pre-collision velocity.

The model implementations have been validated through three different two-dimensional simulation cases: (i) Non-ablating temperature equilibrium tests (square and circle geometries) that demonstrate a physically consistent temperature development over time and a stagnation temperatures in line with order-of-magnitude estimates, (ii) direct comparison to the prior model by [1] shows lower recession rates and a physically more plausible geometry recess (rounded corners, restored symmetry), rather than concave faces with sharp edges obtained by the previous model, (iii) experimental validation against the plasma wind-tunnel ablation tests of Löhle, Hermann, and Zander [3] for the ZURAM probe yields recession rates of $45 - 114\ \mu m\,s^{-1}$(simulation), matching the order of magnitude of the experimentally measured $43\ \mu m\,s^{-1}$. This shows a significant improvement in modeling accurate recession rates compared to the results obtained with the prior ablation model by [1], which were off by a few orders of magnitudes. The convective and radiative heat-flux fall within experimental uncertainties. The remaining discrepancies in the modeled heat transfer mechanisms between simulation and experiment are consistent with the current omission of solid-material heat conduction and pyrolysis effects, such as out-blowing gases.

Overall, the incorporated implementation of local temperature-based surface radiation brings SPARTA's ablation simulations closer to the experimental data and yields a physically more plausible surface evolution. These advances provide a practical foundation for further integration of heat conduction, pyrolysis, and chemical effects into SPARTA's ablation model. This work provides a next step toward realistic ablation recess modeling at early stages of re-entry at high altitudes enabling improved TPS designs and realistic heat-balance modeling.

ACKNOWLEDGEMENTS

The authors like to acknowledge the Leibnitz Super-Computing Center (LRZ) for providing computational and data resource services without which this project would not have been possible.

REFERENCES

[1] L. Bott, *Numerical and Physical Improvements to the Hypersonic Ablation Model in SPARTA* (Master thesis, Technical University of Munich, 2024).
[2] S. Chen, C. Gan, L. Bott, C. Stemmer, J. Zhang, *Journal of Spacecraft and Rockets* **62**, 1101–11087 (2025).
[3] S. Löhle, T. Hermann, F. Zander, *CEAS Space Journal* **10**, 203–2116 (2018).

Abstract 61

Pressure Profile Simulation in the Neutral Beam Injector System of a Volumetric Neutron Source

X. Luo[1,a)], C. Tantos[1], S. Hanke[1], T. Giegerich[1], and T. Haertl[2]

[1] *Karlsruhe Institute of Technology, Institute for Technical Physics, 76021 Karlsruhe, Germany.*
[2] *EUROfusion Consortium, FTD Department, Boltzmannstr. 2, 85748 Garching, Germany.*

[a)] Corresponding author: Xueli.Luo@kit.edu

The Volumetric Neutron Source (VNS) tokamak, which is characterized by its small size, low power and low tritium consumption, is intended to be an important step between the International Thermonuclear Experimental Reactor (ITER) and the European DEMOnstration power plant (EU-DEMO) [1]. Four Neutral Beam Injector (NBI) systems are foreseen to provide ~ 42 MW of heating power to the confined plasma and to ensure steady-state operation in the VNS. Consequently, neutrons are predominantly generated via D-T nuclear fusion reactions to serve as a testbed for fusion in-vessel components, in particular the breeding blanket [2-3].

A comprehensive simulation model has been developed, incorporating all key components of the VNS-NBI. The gas input to the neutralizers and the gas load from the residual ion dumps are considered independently. The vacuum system of the VNS-NBI was systematically simulated with our in-house Test Particle Monte Carlo simulation code ProVac3D, which has been cross-checked and used in many nuclear fusion applications [4-5]. The simulations were carried out on the EUROfusion HPC supercomputer Leonardo at Cineca, utilizing 2000 cores in parallel to process 10^{11} test particles. Pressure profiles along the beamline were obtained via Monte Carlo simulations by varying the capture factor of the pumping surface as shown in Figure 1. These results are crucial for verifying the feasibility of the pumping concept for the VNS-NBI design.

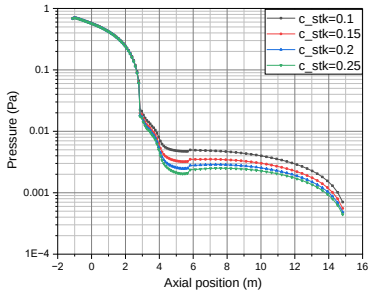


Fig. 1. Pressure profile along the beamline of the NBI system of the VNS.

ACKNOWLEDGEMENTS

This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No. 101052200—EUROfusion). Views and opinions expressed are, however, those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them. The authors acknowledge EUROfusion for the computing resources allocated to project VAC_ND on the supercomputer hosted by CINECA (Italy).

REFERENCES

[1] G. Federici, Nucl. Fusion **63**,125002 (2023).
[2] L. Giannini et al., IEEE Trans. Appl. Supercond. **34(5)**, 4204206 (2024).
[3] T. Haertl, C. Bachmann, T. Franke, B. Heinemann, C. Hopf, G. Janeschitz and M. Siccinio, Fusion Eng. Des. **213**, 114864 (2025).
[4] X. Luo, M. Scannapiego, C. Day, and S. Sakurai, Fusion Eng. Des. **136**, 467(2018).
[5] X. Luo, Y. Kathage, T. Teichmann, S. Hanke, T. Giegerich, and C. Day, Energies **17**, 3889 (2024).

Modeling of Chemically Reactive Gas Flows for Multi-Scale Problems

F. Tuttas[a] and M. Pfeiffer

Institute of Space Systems, University of Stuttgart, Pfaffenwaldring 29, 70569 Stuttgart, Germany

[a]Corresponding author: tuttasf@irs.uni-stuttgart.de

For multi-scale gas kinetic problems, such as re-entry flows, a thorough understanding of the underlying physical processes is essential. In high-temperature environments relevant to space applications, chemical reactions such as the dissociation of molecular oxygen and nitrogen cannot be neglected. Accurate modeling of chemically reactive gases therefore plays a key role in the investigation of these flows.

The Direct Simulation Monte Carlo (DSMC) [1] method provides highly accurate solutions for such flows. However, its computational cost becomes prohibitive in the transition and continuum regimes. Hybrid approaches based on coupling DSMC with computational fluid dynamics (CFD) are challenging due to the fundamentally different nature of the methods, particularly the stochastic particle noise inherent to DSMC.

As a result, particle-based continuum methods employing the Bhatnagar-Gross-Krook (BGK) [2] or Fokker-Planck (FP) [3] approximations have gained increasing attention in recent years. These approaches improve computational efficiency in low-Knudsen regimes by modeling relaxation processes rather than binary collisions, while retaining the particle approach that enables straightforward coupling with DSMC.

In the last years, different continuum-based models in the open-source particle code PICLas [4, 5] have been extended to simulate gas mixtures with internal energy modes [6]. More recently, the Ellipsoidal Statistical BGK (ESBGK) [7] model has been further developed to account for chemically reactive gas mixtures [8]. The present work focuses on improved modeling of chemical reactions in the ESBGK and Shakhov BGK (SBGK) [9] models, with validation through mutual comparison and DSMC simulations. Model accuracy and performance are assessed for several test cases, including reactive gases confined in a reservoir and an application case related to space re-entry.

ACKNOWLEDGEMENTS

This work is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 516238647 – SFB 1667/1 (ATLAS - Advancing Technologies of Very Low-Altitude Satellites)

REFERENCES

[1] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Oxford University Press, New York, 1994).
[2] P. L. Bhatnagar, E. P. Gross, M. Krook, *Phys. Rev.* **94**, 511–525 (1954).
[3] P. Jenny, M. Torrilhon, S. Heinz, *J. Comput. Phys.* **229**, 1077–1098 (2010).
[4] S. Fasoulas, C.-D. Munz, M. Pfeiffer, J. Beyer, T. Binder, S. Copplestone, A. Mirza, P. Nizenkov, P. Ortwein, W. Reschke, *Phys. Fluids* **31**, 072006 (2019).
[5] M. Pfeiffer, *Phys. Fluids* **30**, 106106 (2018).
[6] F. Hild, M. Pfeiffer, *J. Comput. Phys.* **514**, 113226 (2024).
[7] H. L. Holway Jr., *Phys. Fluids* **9**, 1658–1673 (1966).
[8] F. Tuttas, M. Pfeiffer, *3rd International Conference on Flight Vehicles, Aerothermodynamics and Re-entry (FAR)* (Arcachon, France, 2025).
[9] E. M. Shakhov, *Fluid Dyn.* **33**, 95–96 (1968).

Abstract 63

Analysis of Aerodynamic Characteristic Variations with Altitude for a Rocket in Continuum and Rarefied Flow Regimes

Y. Kim[1,a)], and K. T. Kang[1]

[1] *Agency for Defense Development, Dajeon, Republic of Korea*

[a)] Corresponding author: yjkim0426@gmail.com

Understanding the variations in aerodynamic characteristics across different altitudes is fundamental for ensuring the predictable performance and stability of flight configurations operating in diverse atmospheric layers[1]. As a vehicle traverses from the dense lower atmosphere to the rarefied upper atmosphere, the drastic changes in gas density and molecular behavior significantly alter the aerodynamic load distribution. Therefore, accurate characterization of aerodynamic coefficients is essential for vehicles operating over a wide range of altitudes, where flow regimes transition from continuum to rarefied conditions. This study aims to provide comprehensive characterization of the aerodynamic coefficients and stability for a simple con-cylinder body across an altitude range from sea level to 120 km. To capture the distinct physics of these atmospheric layers, a dual numerical simulation was established: Computational Fluid Dynamics (CFD) based on the Navier-Stokes equations was employed for the continuum regime (0–60 km), while the Direct Simulation Monte Carlo (DSMC) method, which provides a stochastic solution to the Boltzmann equation, was utilized for the rarefied regime (80–120 km).

The analysis was conducted at Mach 4 and 6, with angles of attack ranging from 0° to 15°. The results reveal a distinct dependence of aerodynamic coefficients on altitude. In the continuum regime (0–60 km), the normal force coefficients and pitching moment coefficients remain relatively constant, indicating the center of pressure is relatively insensitive to altitude changes within this lower range. However, the axial force coefficient exhibits a steady increase with altitude even in this lower range, primarily due to the decreasing Reynolds number and the resulting rise in skin friction drag. As the altitude exceeds 60 km and enters the transitional and rarefied regimes, a significant upward trend is observed across all aerodynamic coefficients. The most dramatic variations occur between 80 km and 100 km, where the rarefaction of the gas leads to a thickened boundary layer and a fundamental shift in molecular momentum transfer. Furthermore, the longitudinal stability analysis shows that the center of pressure shifts progressively rearward as altitude increases. This shift is a critical consideration for the aerodynamic design and stability prediction of bodies operating across multiple atmospheric layers.

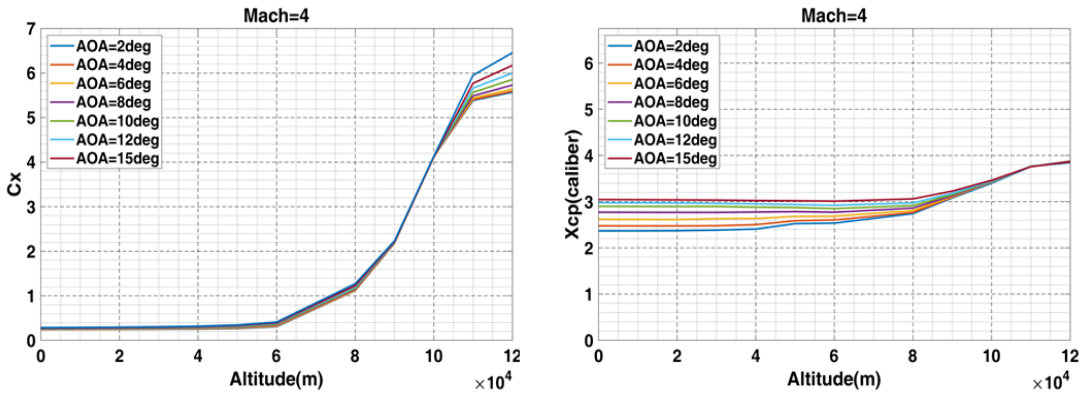


Fig. 1. Variation of the axial force coefficient(Cx) and center of pressure(Xcp) with altitude

REFERENCES

[1] J. N. Moss, C. E. Glass, F. A. Greene, AIAA 2006-3577, pp. 1-18 (2006).

Abstract 64

A Multi-Temperature ES-BGK Model with a Continuous Internal-Energy Variable: Derivation of a Maximum-Entropy 21-Moment System and Two-Temperature Navier–Stokes–Fourier Limits

T. Arima[1,a)], A. Pollino[2]

[1] *National Institute of Technology, Tomakomai College.*
[2] *Technische Universität Wien.*

[a)] Corresponding author: arima@tomakomai-ct.ac.jp

Rarefied polyatomic gases exhibit complex non-equilibrium among translational, rotational, and vibrational modes. To accurately describe shock structures and wave attenuation, a consistent hierarchy connecting kinetic equations to reduced fluid models is essential.

In this study, we propose a multi-temperature ES-BGK model that generalizes the formulation in [1] by introducing a continuous internal-energy variable. This enables a compact description with separate rotational and vibrational relaxation channels, in the spirit of the kinetic model in [2], while retaining realistic transport behavior through the ES-BGK mechanism.

We then derive a consistent moment system from this kinetic model. By applying the maximum entropy principle, we obtain a closed 21-moment system that admits a symmetric-hyperbolic formulation. The field variables consist of mass density, velocity, three distinct mode temperatures (translational, rotational, vibrational), the deviatoric stress, and three heat fluxes associated with translational, rotational, and vibrational energies.

Finally, we analyze the 21-moment system using the order-of-magnitude method [3]. We consider two asymptotic limits based on the hierarchy of relaxation time scales: (i) the regime where translational and rotational modes equilibrate rapidly; and (ii) the regime where rotational and vibrational modes are strongly coupled. We show that the resulting reduced equations recover the two-temperature Navier–Stokes–Fourier (NSF) models of [4–6] as limiting cases under appropriate relaxation-time orderings, thereby providing a unified kinetic-to-continuum route for two-temperature NSF modeling.

ACKNOWLEDGEMENTS

The work of T.A. was partially supported by JST, PRESTO Grant Number JPMJPR23O1, and by JSPS KAKENHI, Grant Numbers JP22K03912, Japan.

REFERENCES

[1] T. Arima, A. Mentrelli, T. Ruggeri, *J. Stat. Phys.,* **191**, 95 (2024).
[2] T. Arima, T. Ruggeri, M. Sugiyama, *Phys. Rev. E*, **96**, 042143 (2017).
[3] H. Struchtrup, *Phys. Fluids*, **16**, 3921–3934 (2004).
[4] E. Kustova, M. Mekhonoshina, A. Kosareva, *Phys. Fluids*, **31**, 046104 (2019).
[5] K. Aoki, M. Bisi, M. Groppi, S. Kosuge, *Phys. Rev. E*, **102**, 023104 (2020).
[6] B. Rahimi, H. Struchtrup, *Phys. Fluids*, **26**, 052001 (2014).

A Navier Type Boundary Condition for Boltzmann Equation

K. Aoki[1], **V. Giovangigli**[2], F. Golse[3] and S. Kosuge[4]

[1]*Department of Mathematics, National Cheng Kung University, Tainan 70101, Taiwan.*
[2]*CMAP, CNRS, Ecole polytechnique, 91128 Palaiseau Cedex, France.*
[3]*CMLS, Ecole polytechnique, 91128 Palaiseau Cedex, France.*
[4]*Institute for Liberal Arts and Sciences, Kyoto University, Kyoto 606-8501, Japan.*

[a)]Corresponding author: vincent.giovangigli@polytechnique.edu

Boundary conditions for the Boltzmann equation at solid-gas interfaces may be investigated by using kinetic equations describing gas particles interacting with a steady wall potential and colliding with phonons describing the fluctuating part of the surface potential [1–5]. We consider such a kinetic equation in a *rescaled* form

$$\partial_t f + \boldsymbol{c}_{\shortparallel} \cdot \boldsymbol{\partial}_{\shortparallel} f + \frac{1}{\epsilon} c_z \, \partial_\zeta f - \frac{1}{\epsilon} \partial_\zeta \mathrm{w} \, \partial_{c_z} f = J(f,f) + \frac{1}{\epsilon} \frac{1}{\tau_{\mathrm{ph}}} (\langle f \rangle M - f),$$

where t is time, $\boldsymbol{x} = (\boldsymbol{x}_{\shortparallel}, z)^t$ the spatial coordinates, $\boldsymbol{\partial}_{\shortparallel}$ the tangential differential, ∂_ζ the normal differential with respect to the layer coordinate $\zeta = z/\epsilon$, f the physisorbate/gas particle distribution function, $\boldsymbol{c} = (\boldsymbol{c}_{\shortparallel}, c_z)^t$ the gas particle velocity, $\mathrm{w} = \mathrm{w}(\zeta)$ the interaction potential with a planar interface located at $\zeta = 0$, J the gas collision operator, $\langle f \rangle = \int f d\boldsymbol{c}$ the number density, $(\langle f \rangle M - f)/\tau_{\mathrm{ph}}$ the gas-phonon collision operator taken in relaxation form, τ_{ph} the relaxation time, and M the wall Maxwellian. This kinetic scaling [4, 5] differs from the fluid scalings used in previous work [2, 3]. The potential w is such that $\lim_{\zeta \to 0} \mathrm{w}(\zeta) = +\infty$, $\lim_{\zeta \to +\infty} \mathrm{w}(\zeta) = 0$, and involves attractive and repulsive zones as Lennard-Jones potentials integrated over the solid body. The phonon interaction time $\tau_{\mathrm{ph}} = \tau_{\mathrm{ph}}(\zeta)$ is such that $\lim_{\zeta \to \infty} \tau_{\mathrm{ph}}(\zeta) = \infty$ and is an increasing function of ζ in $[0, +\infty)$ with a finite positive $\tau_{\mathrm{ph}}(0)$ and $1/\tau_{\mathrm{ph}}(\zeta)$ is integrable over $[0, +\infty)$.

Denoting by $\mathcal{H}(\phi) = c_z \, \partial_\zeta \phi - \partial_\zeta \mathrm{w} \, \partial_{c_z} \phi + (\phi - \langle \phi \rangle M)/\tau_{\mathrm{ph}}$ the operator associated with the thin physisorbate layer equation, then for appropriate inflow distribution $\phi^{\mathrm{in}}(\boldsymbol{c})$, $c_z < 0$, and right hand side $\psi(\zeta, \boldsymbol{c})$, there exists a unique solution $\phi(\zeta, \boldsymbol{c})$ such that $\mathcal{H}(\phi) = \psi$ and $\lim_{\zeta \to \infty} (\phi - \phi^{\mathrm{in}}) = 0$ for $c_z < 0$. This solution ϕ may be written $\phi = \mathcal{G}^{\mathrm{in}} \phi^{\mathrm{in}} + \mathcal{G} \psi$ where the operators $\mathcal{G}^{\mathrm{in}}$ and $\mathcal{G}$ are such that $\mathcal{H}(\mathcal{G}^{\mathrm{in}} \phi^{\mathrm{in}}) = 0$ with $\lim_{\zeta \to \infty} (\mathcal{G}^{\mathrm{in}} \phi^{\mathrm{in}} - \phi^{\mathrm{in}}) = 0$ for $c_z < 0$ as well as $\mathcal{H}(\mathcal{G}\phi) = \psi$ with $\lim_{\zeta \to \infty} \mathcal{G}\phi = 0$ for $c_z < 0$. Introducing the limit operator $\mathcal{G}^{\mathrm{in}}_\infty = \lim_{\zeta \to \infty} \mathcal{G}^{\mathrm{in}}$ for $c_z > 0$ then $\mathcal{G}^{\mathrm{in}}_\infty \phi^{\mathrm{in}}$ yields the corresponding distribution outflowing the physisorbate. The zeroth order boundary condition for Boltzmann equation in the gas may then be written in the form $f_{\mathrm{g}}^{(0)} = \mathcal{G}^{\mathrm{in}}_\infty f_{\mathrm{g}}^{(0),\mathrm{in}}$ for $c_z > 0$ [4, 5]

We define $\mathcal{G}'\phi = \mathcal{G}\big(\mathcal{G}^{\mathrm{in}}(c_z \phi) - c_z \phi + \zeta \partial_\zeta \mathrm{w} \, \partial_{c_z} \phi - \big(\phi - \langle \phi \rangle M \big) \big)/\tau_{\mathrm{ph}}$ and $\mathcal{L}\phi = \mathcal{G}(\mathcal{G}^{\mathrm{in}}(J(\phi,\phi)) - J(\mathcal{G}^{\mathrm{in}}\phi, \mathcal{G}^{\mathrm{in}}\phi))$ and the limits $\mathcal{G}'_\infty = \lim_{\zeta \to \infty} \mathcal{G}'$ and $\mathcal{L}_\infty = \lim_{\zeta \to \infty} \mathcal{L}$ for $c_z > 0$. The first order distribution outflowing in the gas f_{g} for $c_z > 0$, that yields a first order boundary condition for Boltzmann equation in the gas, satisfies

$$f_{\mathrm{g}} = \mathcal{G}^{\mathrm{in}}_\infty f^{\mathrm{in}}_{\mathrm{g}} + \epsilon \, \mathcal{G}'_\infty \partial_z f_{\mathrm{g}} + \epsilon \, \mathcal{L}_\infty f_{\mathrm{g}}, \qquad c_z > 0,$$

where $f^{\mathrm{in}}_{\mathrm{g}} = f_{\mathrm{g}}$ for $c_z < 0$ is the first order distribution inflowing in the physisorbate from the gas $f^{\mathrm{in}}_{\mathrm{g}} \approx f^{(0),\mathrm{in}}_{\mathrm{g}} + \epsilon f^{(1),\mathrm{in}}_{\mathrm{g}}$. The term $\mathcal{G}^{\mathrm{in}}_\infty f^{\mathrm{in}}_{\mathrm{g}}$ is thus similar to that at zeroth order but naturally involves the first order gas distribution $f^{\mathrm{in}}_{\mathrm{g}}$ infolwing in the physisorbate, the new term $\epsilon \mathcal{G}'_\infty \partial_z f_{\mathrm{g}}$ is a first order nonlocal Navier type correction and $\epsilon \mathcal{L}_\infty f_{\mathrm{g}}$ is a nonlinear correction due to collisions in the physisorbate.

REFERENCES

[1] V.D. Borman, S.Yu. Krylov, and A.V. Prosyanov, *Theory of nonequilibrium phenomena at a gas-solid interface*, JETP **67**, 2110–2121 (1988).
[2] K. Aoki and V. Giovangigli, *Kinetic model of adsorption on surfaces*, Phys. Rev. E **99**, 052137 (2019).
[3] K. Aoki and V. Giovangigli, *Kinetic theory of chemical reactions on surfaces*, Physica A **565**, 125573 (2021).
[4] K. Aoki, V. Giovangigli, and S. Kosuge, *Boundary conditions for the Boltzmann equation from gas-surface interaction kinetic models*, Phys. Rev. E **106**, 035306 (2022).
[5] K. Aoki, V. Giovangigli, F. Golse and S. Kosuge, *The Physisorbate-Layer Problem Arising in Kinetic Theory of Gas-Surface Interaction*, J. Stat. Mech., **191** 53 (2024).

An Accurate Energy-Preserving Particle Integration Scheme for the Vlasov-Fokker-Planck System

A. Riess[1,a)], H. Gorji[2] and P. Jenny[1]

[1]*ETH Zurich, Switzerland*
[2]*EMPA, Switzerland*

[a)]Corresponding author: ariess@ethz.ch

We present a novel energy-preserving time integration scheme for simulations of interacting charged particles in electromagnetic fields. Coulomb interactions between particles are modelled using a Fokker-Planck collision operator, while external forces arise from a prescribed electromagnetic field, resulting in a Vlasov-Fokker-Planck description of the particle dynamics.

A previously proposed time integration method provides an exact solution in the case of a constant electric and magnetic fields. This property offers a substantial computational advantage, enabling significantly larger time steps compared to classical approaches such as the widely used Boris scheme. However, when the electromagnetic fields are spatially or temporally inhomogeneous, the integration is no longer exact, and maintaining energy conservation becomes a critical issue in many applications.

In this work, we extend the existing particle integration scheme to enforce exact energy conservation. In the collision-less setting, the energy of each particle is preserved by iteratively correcting its position and velocity based on the local electric field. In the presence of collisions, however, particles exchange energy through Coulomb interactions, and individual particle energies are no longer conserved. In this case, energy conservation is enforced in a weak sense through an appropriate correction procedure.

Abstract 67

Aerothermal Comparisons of CFD and Flight Data for the W-2 Reentry Capsule Using the MMT Model

S. R. Cranford[1,a)], T. J. Gross[1], and T. E. Schwartzentruber[2]

[1] *Department of Aerospace Engineering and Mechanics, University of Minnesota, Minneapolis, MN 55455*

[a)] Corresponding author: cranf014@umn.edu

Varda Space Industries' W-2 reentry capsule successfully flew an onboard optical emissions spectrometer taking in situ shock layer measurements at hypervelocity conditions along its trajectory between 105 to 50 km [1]. Computational fluid dynamic (CFD) and direct simulation Monte Carlo (DSMC) analysis of the W-2 flight was performed by Crespo et al. [2] and Valentini et al. [3]. For CFD with traditional Park 11 species air with Millikan and White vibrational relaxation, Crespo et al. [2] observed synthetic spectral radiance levels higher than those measured by the onboard spectrometer [1], when using NASA's High-temperature Aerothermodynamic Radiation Algorithm (HARA) code. However, when Valentini et al. [3] performed DSMC with reaction rates and vibrational relaxation times informed by first-principles air chemistry data, they observed better agreement between the flight data and synthetic spectral radiance. This work compares CFD performed with the Modified Marrone-Treanor (MMT) air chemistry model [4,5] for the Varda W-2 reentry capsule to the measured flight data [1] and DSMC of Valentini et al. [3] for the 58 and 78 km trajectory points. Additionally, the effect of including full multicomponent diffusion is assessed as well as continuum breakdown effects utilizing a slip-wall model in the CFD simulations [6].

ACKNOWLEDGEMENTS

This work was funded by the United States Air Force Research Laboratory, Space Vehicles Directorate (Civilian Academic Degree Program) and the Air Force Office of Scientific Research (grant FA9550-23-1-0446). The views and conclusions are those of the authors and should not be interpreted as representing official policies or endorsements of the U.S. Government.

REFERENCES

[1] A. P. Rao, J. D. Crespo, P. Valentini, V. J. Murray, E. I. Vaughan, Z. S. Davis, R. Alviani, M. Kulakhmetov, Journal of Spacecraft and Rockets, (December 2025), pp. 1–14.
[2] J. D. Crespo, P. Valentini, A. Rao, Z. S. Davis, C. O. Johnston, Proc. of the AIAA SCITECH 2026 Forum (American Institute of Aeronautics and Astronautics, Orlando, FL, 2026).
[3] P. Valentini, Z. S. Davis, J. D. Crespo, A. P. Rao, Acta Astronautica (January 2026), submitted.
[4] R. S. Chaudhry, E. Torres, T. E. Schwartzentruber, G. V. Candler, "Modified Marrone-Treanor Dissociation Model: Formulation and Benchmarking for Diatom/Atom Mixtures," 2025.
[5] E. Torres, T. Gross, G. V. Candler, T. E. Schwartzentruber, "Parameterization and Benchmarking of the Modified Marrone-Treanor Model for Five-Species Air," 2025.
[6] S. R. Cranford, M. D. Kroells, T. J. Gross, T. E. Schwartzentruber, Proc. of the AIAA SCITECH 2026 Forum (American Institute of Aeronautics and Astronautics, Orlando, FL, 2026).

Modeling Reacting Flow for Hybrid Navier-Stokes/DSMC Methods

Mitchell Wall[1,a)] and Iain D. Boyd[1]

[1]*Ann and H.J. Smead Department of Aerospace Engineering Sciences, University of Colorado Boulder, Boulder, Colorado 80303, USA.*

[a)]Corresponding author: mitchell.wall@colorado.edu

Modeling transitional Knudsen number flow remains a significant challenge in hypersonics. In this regime, continuum methods such as the Navier–Stokes (NS) equations lose accuracy, requiring the use of more computationally expensive methods such as Direct Simulation Monte Carlo (DSMC) [1]. To address this challenge, this work employs the Modular Particle–Continuum (MPC) method [2], which is designed to bridge the transitional regime. The MPC framework decomposes the flow field into continuum and particle domains, allowing computationally less expensive CFD methods to be used where physically accurate, while applying DSMC only in regions where it is necessary. MPC can currently model 2D flows of gas mixtures with translational, rotational, and vibrational nonequilibrium.

One limitation of the MPC method is the omission of chemical reactions. Chemical reactions can act as a significant energy sink even within the transitional regime and should be included. Building on work from Holman [3], modifications are made to standard NS and DSMC chemistry calculations for MPC to improve consistency between the two methods. Figure 1 shows a zero-dimensional adiabatic reactor of N_2 dissociating in time. The NS and DSMC chemistry models show good agreement, indicating that they are suitable for use within MPC.

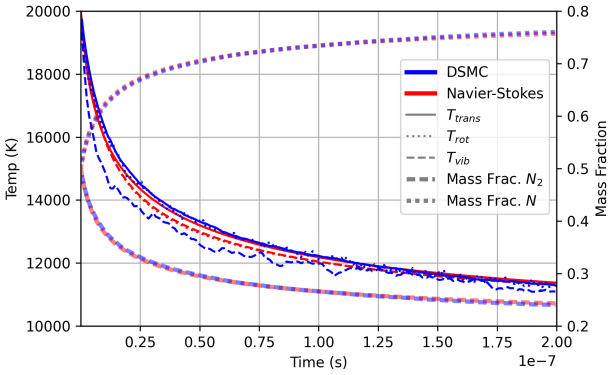


Fig. 1: Zero-dimensional adiabatic reactor of N_2 dissociating in time compared between NS and DSMC calculations.

Building on the demonstrated similarity of zero-dimensional MPC chemistry models, this work will focus on flow quantities in two-dimensional flow fields. The development, performance, and accuracy of this approach will be examined. Agreement between particle and continuum solutions will be quantified, and results will be verified against full DSMC and CFD simulations to assess both computational performance and physical accuracy.

ACKNOWLEDGEMENTS

The first author gratefully acknowledges funding from the Department of Defense National Defense Science and Engineering Graduate Fellowship (DoD NDSEG) and the Smead Program at the University of Colorado Boulder.

REFERENCES

[1] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Clarendon Press, Oxford, UK, 1994).

[2] T. E. Schwartzentruber, L. C. Scalabrin, I. D. Boyd, *Journal of Computational Physics* **225**, 1159–1174 (2007).

[3] T. Holman, "Numerical investigation of the effects of continuum breakdown on hypersonic vehicle surface properties," Ph.D. thesis, University of Michigan 2010.

An Inverse-Design Approach to Characterizing Gas-Surface Interaction in VLEO and Their Effects on Aerodynamic Drag

S. S. Ramesh[1,a)], B. Y. J. Wong,[1], W. L. Chan[2] and R. Y. Tay[3]

[1]*Temasek Laboratories, National University of Singapore, Singapore 117411.*
[2]*Singapore University of Technology and Design, Singapore, 487372.*
[3]*Temasek Laboratories, Nanyang Technological University, Singapore 637553.*

[a)]Corresponding author: tslssr@nus.edu.sg

Operating satellites in VLEO is challenged by severe atmospheric drag, exacerbated by atomic oxygen (AO) erosion. While molecular beam experiments provide crucial scattering data [1], a gap remains in translating these findings into predictive simulations which require specification of Gas-Surface Interaction (GSI) coefficients. Standard GSI scattering models like the Cercignani, Lampis and Lord (CLL) model fail to reproduce experimental distributions. Furthermore, while advanced models like the modified Washboard model [2] capture experimental distributions more accurately, their implementation for complex geometries in standard TPMC/DSMC frameworks remains a significant challenge, thus necessitating a different approach. This study leverages an inverse-design approach to characterize GSI coefficients using two distinct modeling techniques: the "Weighted CLL" (WCLL) and the "Scaled CLL" (SCLL). These coefficients are determined by calibrating the models against the experimental data of Minton et al. [1], after which their respective impacts on predicted drag reduction are compared. Preliminary results indicate that while the WCLL model reasonably captures energy distribution, drag reduction is overestimated by 10 – 20% relative to the SCLL. The SCLL model provides a better quantitative match with experimental data but introduces a non-physical scaling artifact. Despite these individual limitations, both models successfully capture relative difference in drag between coated and diffuse surfaces, especially at grazing incidence angles as illustrated in Fig.1 for a wedge shaped ram face with different GSI specifications. The next phase of this research will involve propagating a satellite's orbit in VLEO environment using these newly characterized GSI coefficients, allowing us to quantify how predicted "drag reduction" translates into tangible mission benefits, such as propellant savings and extended operational lifetime.

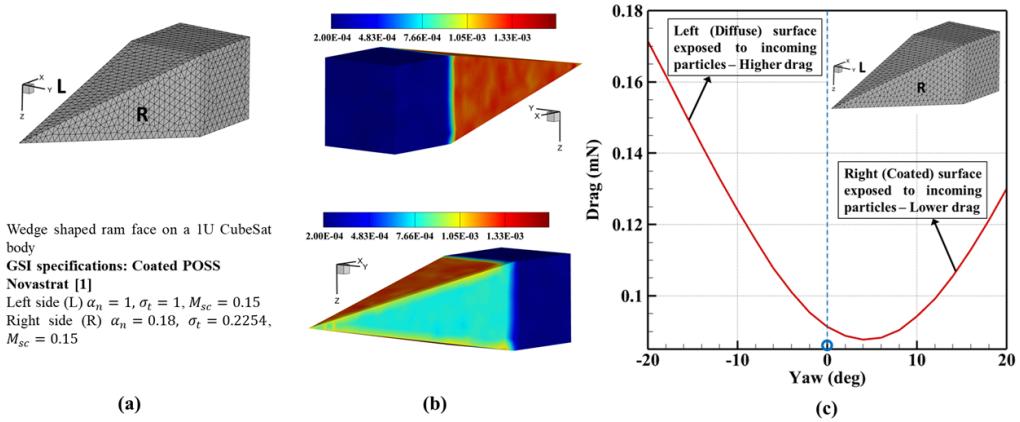


Fig. 1. (a) Satellite model (wedge height/base = 3) with variable GSI specification, (b) Normal pressure distribution (Pa) on left and right surfaces at yaw = 0° and (c) Drag variation with yaw angle (exposing different surfaces to incoming particles.)

ACKNOWLEDGEMENTS

This study is funded by the Office of Space Technology and Industry, Singapore, under grant S24-020025-STDP. The computational work for this paper is fully supported by NUS IT's Research Computing group under grant number CFP01-CF-057.

REFERENCES

[1] T. K. Minton, T. E. Schwartzentruber, C. Xu, *ACS Appl Mater Interfaces* **13**, 51673–51684 (2021).
[2] P. D. C. Jorge, T. E. Schwartzentruber, A. Hubin, T. E. Magin, T. K. Minton, *The Journal of Physical Chemistry C* **129**, 12486–12501 (2025).

A Unified Physical-Neural Modeling Framework for Rarefied Gas Dynamics via Differentiable Simulation

T. Xiao[1,2,a)]

[1]*Institute of Mechanics, Chinese Academy of Sciences, Beijing, China*
[2]*School of Engineering Science, University of Chinese Academy of Sciences, Beijing, China*

[a)]Corresponding author: txiao@imech.ac.cn

Modeling and simulation of rarefied gas dynamics often involve parameter calibration, model design, and inverse analysis, yet the application of gradient-based optimization in kinetic solvers remains limited due to the complexity of classical adjoint derivations and nonlinear multi-scale couplings. In this work, we present a novel differentiable solution algorithm for rarefied gas dynamics. The central idea is to construct a numerical solver whose entire computational procedure—discretization, iteration, and time integration—is differentiable, enabling the direct computation of gradients of physical quantities with respect to model parameters through automatic differentiation [1]. This approach bypasses manually derived adjoint systems and establishes a unified framework in which numerical simulation and gradient-based optimization are seamlessly integrated.

The differentiable simulator further enables a unified physical–neural modeling paradigm. Neural network components can be embedded into kinetic solvers to represent closure relations, collision operators, or surrogate modules, while their parameters are optimized end-to-end via gradients propagated through the full simulation program. This framework supports forward simulation, inverse problems, and data-driven model refinement within a single computational infrastructure. Numerical experiments on the Boltzmann equation and its moment systems demonstrate the effectiveness, flexibility, and significant computational acceleration achievable by the proposed method. The reproducible implementation is available in the open-source Julia package Kinetic.jl [2].

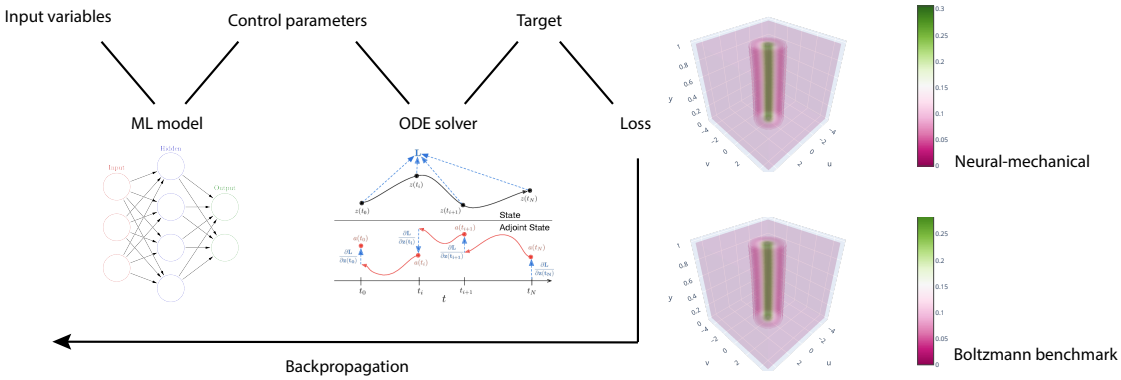


Fig. 1. Left: schematic of differentiable simulation that incorporates numerical solver and machine learning models; Right: comparison of simulation results using the physical-neural model and the Boltzmann equation along the vertical central line in three-dimensional lid-driven cavity flow.

ACKNOWLEDGEMENTS

The current work is funded by German Research Foundation (SPP2298-441826958) and National Natural Science Foundation of China (12302381, 2572340).

REFERENCES

[1] S. Cuomo, V. S. Di Cola, F. Giampaolo, G. Rozza, M. Raissi, F. Piccialli, *Journal of Scientific Computing* **92**, 88 (2022).
[2] T. Xiao, *Journal of Open Source Software* **6**, 3060 (2021).

Kinetic theory of sheared granular gases with velocity-dependent inelastic collisions

M. R. Kikuchi[1,a)], Y. Kobayashi,[1] and S. Takada[1,b)]

[1]*Department of Mechanical Systems Engineering, Tokyo University of Agriculture and Technology, 2-24-16 Naka-cho, Koganei, Tokyo 184-8588, Japan*

[a)]m-kikuchi@st.go.tuat.ac.jp
[b)]Corresponding author: takada@go.tuat.ac.jp

We develop a kinetic-theoretical description of sheared rarefied granular gases composed of smooth hard spheres with velocity-dependent inelastic collisions. The model assumes a restitution coefficient that depends on the normal component of the impact velocity and varies discontinuously in a piecewise manner, mimicking multistage energy dissipation mechanisms observed in realistic granular interactions [1]. Despite its simplicity, this collision rule introduces nontrivial nonlinearity into the Boltzmann equation and significantly modifies the collisional moments.

Focusing on steady simple shear flow, we analytically derive the rheological properties of the system, including the shear stress, normal stress differences, and the shear-rate dependence of the effective viscosity. The kinetic equation is solved using a controlled approximation based on Grad's moment method [2], allowing us to explicitly identify how the velocity-dependent inelasticity alters the balance between viscous heating and collisional dissipation. We show that the discontinuous restitution law leads to pronounced non-Newtonian behavior, characterized by shear-thinning or thickening regimes depending on the shear rate and the thresholds defining the collision stages.

Our results demonstrate that even in dilute granular gases, the detailed velocity dependence of inelastic collisions plays a crucial role in determining macroscopic transport properties as shown in Fig. 1. The present framework provides a tractable extension of classical kinetic theories for granular gases and offers a unified description of shear rheology in systems with complex, non-smooth collision rules.

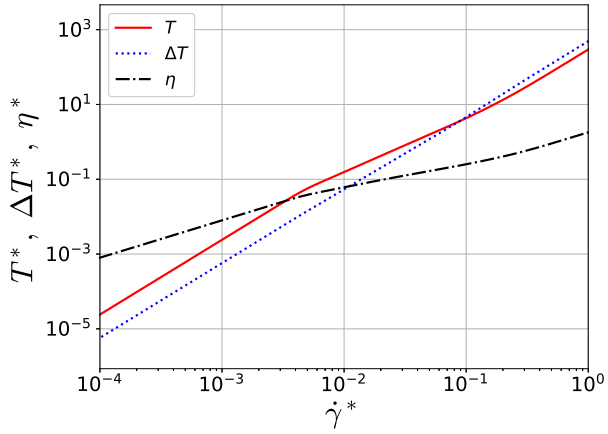


Fig. 1. Shear rate dependence of the dimensionless temperature, anisotropic temperature, and viscosity.

ACKNOWLEDGEMENTS

This work is partially supported by the Grant-in-Aid of MEXT for Scientific Research (Grant No. JP24K06974, No. JP24K07193, and No. JP25K01063).

REFERENCES

[1] T. Pöschel, N. V. Brilliantov, T. Schwager, *Physica A* **325**, 274–283 (2003).
[2] H. Grad, *Commun. Pure Appl. Math.* **79**, 331–407 (1949).

H-theorems for dense reactive mixtures and global existence of solutions

Jacek Polewczak[1,a)]

[1]*Department of Mathematics, California State University, Northridge, CA, 91330, USA*

[a)]Corresponding author: jacek.polewczak@csun.edu

Simple reacting spheres (SRS) model has been developed in [1] and further advanced in [2], [3], and [4], In the SRS model, the molecules behave as if they were single mass points with two internal states of excitation. Collisions may alter the internal states. I consider a dense mixture of four species A, B, A^*, B^*, consisting of hard spheres with diameters d_i and masses m_i, where indices $1, 2, 3, 4$ are for the particles A, B, A^*, B^*, respectively. In contrast to the dilute gas regime, in this work the two-particle distribution function of the mixtures, $f_{ij}^{(2)}$ is approximated (see, H. van Beijeren and M. H.Ernst, *The modified Enskog equation for mixtures*, Physica **70** (1973), 225-242) **not** by $f_{ij}^{(2)} = f_i f_j$ but by $f_{ij}^{(2)} = g_{ij}^{(2)} f_i f_j$, with f_i being a one-particle distribution function of the mixtures and $g_{ij}^{(2)}$ being the pair correlation function of hard spheres at non-uniform equilibrium, with well known algebraic expression. I assume that when a hard-sphere A collides with another hard-sphere B, there is a probability $0 \leq \alpha_R \leq 1$ where in the reaction $A + B \to A^* + B^*$, A^* and B^* are formed. Furthermore, m_i and d_i denote the mass and the diameter of the i-th particle, $i = 1, \ldots, 4$, and reactions take place when the reactive particles are separated by a distance $\sigma_{12} = \frac{1}{2}(d_1 + d_2) = \sigma_{34} = \frac{1}{2}(d_3 + d_4)$ and the kinetic energy associated with the relative motion exceeds the activation energies γ_i: $(1/2)\mu_{is}\Big(\langle \epsilon, v - w\rangle\Big)^2 \geq \gamma_i$, where $\mu_{is} = \frac{m_i m_s}{m_i + m_s}$ are the reduced masses. The conservation of mass has the form $m_1 + m_2 = m_3 + m_4$, where m_i denotes the mass of the i-th particle, $i = 1, \ldots, 4$. The nonlinear kinetic system is

$$\frac{\partial f_i}{\partial t} + v\frac{\partial f_i}{\partial x} = J_i^E + J_i^R, \quad i = 1, 2, 3, 4, \tag{1}$$

where J_i^E are elastic (hard-sphere) collisional operators and J_i^R are reactive collisional terms.
The convergence of the infinite Mayer virial expansion for $g_{ij}^{(2)}$ is not known at present, instead, I consider a truncated series for $g_{ij}^{(2)}$, with finite, but arbitrary number of terms.
First, I show existence of an H-functional for system (1). This is the first such result for **dense reacting** systems. The H-functional: $H(t) = H_B(t) + H_{corr}(t)$ consists of two parts: the kinetic part, $H_B(t) = \sum_{i=1}^{4} \iint f_i \log f_i \, dvdx$, and the correlational part, $H_{corr}(t)$. The structure of $H_{corr}(t)$ is similar to the algebraic structure of the equilibrium (non-uniform) entropy for the mixture of hard–spheres. In addition, one can identify that $-\beta H_{corr} = A^{excess}$ with $\beta = 1/kT$, where A^{excess} is the excess free energy for the mixture hard-spheres in a **non-uniform** equilibrium.

Next, I construct approximate solutions to system (1). Starting with L^1 initial data, I utilize the conservation laws and the H-function to show convergence of the approximate solutions to a solution of system (1). This is the first such existence result for **dense reactive** mixture.

Additionally, when $\alpha_R = 0$ (no reactive terms), system (1) becomes an inert dense mixture of hard spheres (in this case one can consider any number of species with arbitrary masses) and this work also provides the first global in time existence of solutions for such system.

REFERENCES

[1] N. Xystris and J. S. Dahler, J. Chem. Phys. **68** (1978), 387–401)
[2] J. S. Dahler, L. Quin, J. Chem. Phys. **103**, (1995), 725–750
[3] J. S. Dahler, L. Quin, J. Chem. Phys. **118** (2003), 8396–8404).
[4] J. Polewczak, A. J. Soares, Kinetic and Related Models **10** (2017), No. 2, pp. 513 - 539).

Fast-convergence and asymptotic-preserving simulation of charged particle flows based on the Vlasov-BGK-Poisson system

Y. Wen[1,a)] and L. Wu[1]

[1]*Southern University of Science and Technology, China*

[a)]Corresponding author: 12541066@mail.sustech.edu.cn

The simulation of charged particle transport in plasma physics remains a significant computational challenge due to the multi-scale nature of the Vlasov-BGK-Poisson equations, which couple kinetic collision processes with self-consistent electrostatic fields. Macroscopic fluid models, such as the Navier-Stokes equations, fail to accurately describe the non-equilibrium physics in rarefied regimes due to the breakdown of the continuum assumption. However, traditional kinetic numerical methods, such as the Particle-in-Cell with Monte Carlo Collisions and the discrete velocity method, suffer from prohibitive computational costs or extremely slow convergence in the near-continuum (low Knudsen number) regimes.

In this work, we extend the general synthetic iterative scheme to the Vlasov-BGK-Poisson system to achieve fast-convergence and asymptotic-preserving simulations of charged particle flows. By introducing a set of macroscopic synthetic equations derived from the moments of the kinetic equation2̆014incorporating high-order non-equilibrium terms and the self-consistent Poisson coupling2̆014the proposed scheme enables rapid information exchange across both physical and velocity spaces. Numerical results demonstrate that this framework significantly accelerates convergence compared to conventional iterative schemes, achieving an acceleration ratio of nearly two orders of magnitude in the near-continuum limit. Furthermore, the method maintains the asymptotic-preserving property, allowing for the use of coarse spatial grids that do not resolve the molecular mean free path without sacrificing numerical accuracy. This advancement provides an efficient computational tool for the multi-scale modeling of plasma systems

Comparative Analysis of International Space Station Frame Charging Observations from Solar Minimum to Solar Maximum

Gabe R. Wilson[1,a)], Carlos Maldonado[1], Rachel Ulrich[1], Kelly Moran[1], Ky Potter[1] and Lauren Castro[1]

[1] *Los Alamos National Laboratory*
P.O. Box 1663 Los Alamos, NM 87545

[a)] Corresponding author: gwilson@lanl.gov

We present comparative measurements of International Space Station (ISS) frame charge magnitude and rate obtained from two laminated electrostatic analyzers (ESA)[1]: the Autonomous Plume Sentry (APS) [2] and the Electric Propulsion Electrostatic Analyzer Experiment (ÉPÉE) [3]. The charging of the ISS is a multifaceted process influenced by both geomagnetic activity and the conditions of the ionospheric plasma [4]. This electrical charging primarily results from the interaction between the ISS's photovoltaic (PV) array electrical power system (EPS) and the F2 region of the ionosphere. Specifically, the ISS becomes charged due to the collection of electrons on the exposed, positively charged edges of solar cells within its PV arrays. The amount of electron current collected is contingent upon the temperature and density of the ionospheric plasma [5]. These interactions, including both PV array and magnetic induction driven charging, have been extensively studied since the activation of the ISS's 160 V PV arrays in late 2000 [4].

APS and (ÉPÉE) were developed at Los Alamos National Laboratory and the U.S. Air Force Academy. Both employed ram-facing ESAs that collected ion energy spectra, from which plasma density and spacecraft potential were derived. APS also employed a wake-facing instrument, used in this study as a second source of frame charge measurements. Figure 1 shows representative measurements from APS (left panel, May 3, 2017) and 'EP'EE (right panel, March 25, 2023). The top panels display normalized density, while the bottom panels show spacecraft potential. For APS, both ram-facing (blue) and wake-facing (black) ESA measurements are shown.

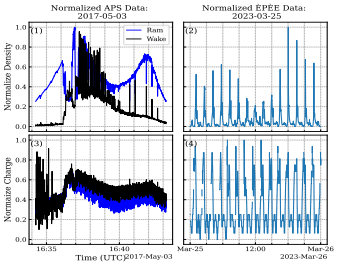


Figure 1. Normalized density (top) and spacecraft potential (bottom) measured by APS (left) ram (blue) and wake (black) ESAs on May 3, 2017, and ÉPÉE (right) on March 25, 2023.

APS operated aboard ISS from February 2017 to July 2018 during the declining phase of Solar Cycle 24, capturing data near solar minimum conditions. ÉPÉE operated from March 2023 to April 2024 during Solar Cycle 25's ascent toward maximum activity. ÉPÉE incorporated improvements over APS including extended energy range, enhanced signal-to-noise ratio, and a laminated collimator that reduced contamination from forward-scattered particles and photons. These enhancements provide improved temporal and energy resolution for characterizing the dynamic ionospheric environment during active solar conditions. In this study, we compare the absolute values and rate of change of the measured frame potential against the measured ion density, spacecraft sun state, and solar activity (sunspot number and F10.7) between the two instruments at the two extremes of the solar cycle. This analysis quantifies how ISS charging behavior varies between solar minimum and solar maximum conditions.

ACKNOWLEDGEMENTS

This work was supported by Los Alamos National Laboratory and the United States Air Force Academy – Space Physics and Atmospheric Research Center, and the US DoD Space Test Program.

REFERENCES

[1] C. A. Maldonado, Z. Eyler, B. Pierce, L. Matson, P. Neal, H. Richards, R. Balthazor, J. Harley, M. McHarg, *Review of Scientific Instruments* **91** (2020).

[2] C. A. Maldonado, A. D. Ketsdever, R. D. Balthazor, P. C. Neal, G. R. Wilson, M. G. McHarg, R. Osiander, R. J. Adams, *Journal of spacecraft and rockets* **60**, 339–350 (2023).

[3] C. A. Maldonado, L. Castro, J. Derr, P. A. Fernandes, K. Moran, T. K. Kim, S. M. Klem, J. Woodroffe, T. Eddy, G. R. Wilson *et al.*, *2025 IEEE Aerospace Conference* (IEEE, 2025), 1–15.

[4] S. Koontz, M. Valentine, T. Keeping, M. Edeen, W. Spetch, P. Dalton, *8th Spacecraft Charging Technology Conference* (2004).

[5] T. L. Morton, D. C. Ferguson, *2001 Pulsed Power Plasma Science Meeting* (2001).

Abstract 79

DSMC Simulations and Ground Tests for ABIE Intake Development

T. Ozawa[1,a)], R. Endo[2], M. Tagawa[3], T. Yamamoto, and S. Imamura[1]

[1] *Japan Aerospace Exploration Agency*
Chofu, Tokyo 182-8522 JAPAN
[2] *Graduate School of Creative Science and Engineering*
Waseda University, Shinjuku-ku, Tokyo 169-8050, JAPAN
[3] *Graduate School of Engineering*
Kobe University, Kobe, Hyogo 657-850, JAPAN

[a)] Corresponding author: ozawa.takashi@jaxa.jp

In order to improve the feasibility of the air breathing ion engine (ABIE) [1] for very low earth orbits (VLEO) satellites [2], a study to improve intake performance for an ion engine μ10 has been carried out at Japan Aerospace Exploration Agency (JAXA). In our previous work,[3] an intake configuration with the ion engine μ 10 has been proposed (see Fig. 1) , and the performance has been analyzed. Also, Shoda *et al.* [4] proposed microstructured surfaces for intake performance improvement. In this work, we first carry out direct simulation Monte Carlo (DSMC) [5] simulations to improve the intake performance estimation in VLEO flight environments by analyzing the influence of layout environments and the effect of microstructured surfaces. Second, we study whether the effect of microstructured surfaces can be observed in Hypersonic Rarefied Wind Tunnel [6] environments.

Keywords: Rarefied Gas Dynamics, Hypersonic Flows, Aerodynamics, DSMC, Air Breathing Ion Engine

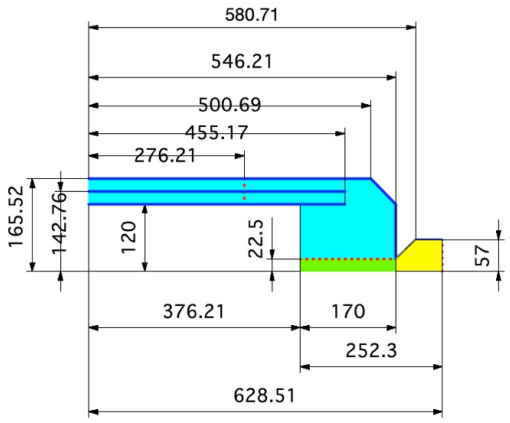


Fig. 1. A proposed intake configuration with an ion engine μ 10.

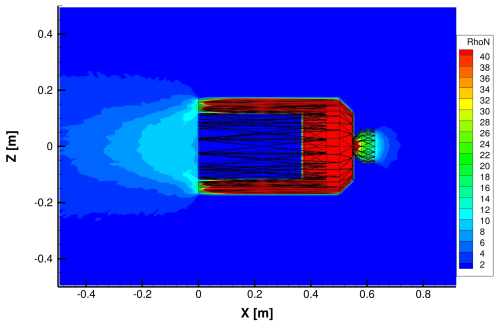


Fig. 2. A normalized density contour plot inside the intake at 268 km (α =0.9, without any exit grids).

ACKNOWLEDGEMENTS

The research performed at JAXA was partly supported by the Grant-in-Aid for Scientific Research (C), No. 24K07893 from Japan Society for the Promotion of Science (JSPS) whose support is gratefully acknowledged.

REFERENCES

[1] Nishiyama, K., *Proceedings of the 54th International Astronautical Congress*, IAC-03-S4-02 (2003).
[2] Sasaki, M., *Space Research Today*, Vol. 198, pp.10-18 (2017).

Abstract 79

[3] Ozawa, T., Imamura, S., Tagawa, M., and Yokota, K., "DSMC Computations of Intake Performance for Air Breathing Ion Engine," 33rd International Symposium on Rarefied Gas Dynamics, July 15-19, 2024, Gottingen, Germany.
[4] Shoda, K., Sakaue, H., and Tagawa, M.: “Enhancement of Inlet Performance in Rarefied Gas Flow Using Micro-structured Surfaces,” CEAS Space Journal, Vol. 15, 2023, pp. 403–411.
[5] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Clarendon, Oxford, England, U.K., 1994.
[6] Ozawa, T., Fujita, K., and Suzuki, T., "Development of an Aerodynamic Measurement System for Hypersonic Rarefied Flows," *Review of Scientific Instruments*, Vol. 86, No. 1, Jan. 2015, 015105

Configuration Optimization of ABEP-Equipped VLEO Satellites Based on a Feasible-Region Approach

C. Yang[1,a)], Y.Hu[2], Jinyue Geng[2], Xiaoqi Li[2], Heji Huang[2] and Quanhua Sun[2]

[1] *Wide-range Flight Engineering Science and Applications Center, Institute of Mechanics, Chinese Academy of Sciences, Beijing, 100190, China*
[2] *State Key Laboratory of High Temperature Gas Dynamics, Institute of Mechanics, Chinese Academy of Sciences, Beijing, 100190, China*

[a)] Corresponding author: yangchao@imech.ac.cn

Very low Earth orbit (VLEO) satellites have been extensively studied over the past two decades due to their potential advantages in space applications such as high-resolution Earth observation and internet constellations. However, rapid orbital decay caused by aerodynamic drag remains a major technical challenge, particularly for long-term missions. Atmosphere-breathing electric propulsion (ABEP) [1], which collects ambient atmospheric molecules and uses them as propellant, can reduce onboard propellant consumption and is therefore considered a promising technology for long-term VLEO missions.

To generate sufficient thrust to overcome aerodynamic drag, ABEP must be supplied with adequate solar power and atmospheric propellant simultaneously [2]. Both capabilities depend on the satellite configuration (see Fig.1): available solar power is mainly determined by the side area of the solar panels and the satellite body, whereas the amount of atmospheric propellant collected is closely related to the frontal area of the satellite body. In addition, aerodynamic drag is also directly related to the satellite's frontal and side areas; the coupled effects of these three factors make configuration optimization challenging.

In this paper, the feasible region of VLEO satellite configuration parameters is derived under constraints on both energy (solar power) and mass (atmospheric propellant). Based on this feasible region, we develop an optimization method for the configuration parameters, which can identify the theoretical optimum (corresponding to minimum drag) as well as engineering design points with thrust margins (see Fig.2).

Finally, by incorporating a previously developed active intake system [3], we obtain optimized configurations for different flight altitudes and payload requirements. The intake configuration is optimized together with the satellite configuration, and the air collection efficiency is dynamically evaluated using Test Particle Monte Carlo (TPMC) simulations and theoretical models. The results show that, for VLEO satellites equipped with an ABEP system, increasing the frontal area and the solar-array area can improve the payload-available power and payload-available volume.

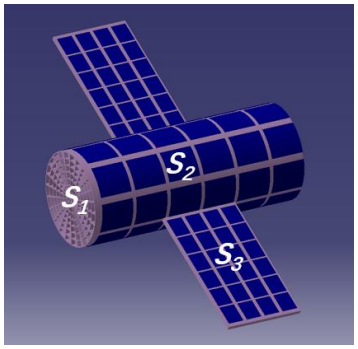


Fig. 1. Schematic of the satellite configuration

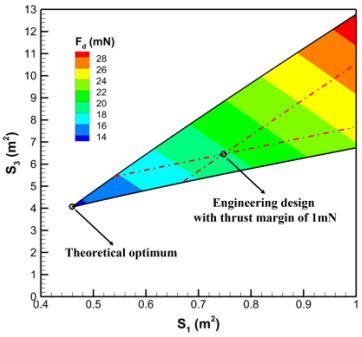


Fig. 2. Feasible region of configuration parameters

ACKNOWLEDGEMENTS

This work was supported by the National Natural Science Foundation of China (Grant No.12202458) and the Strategic Priority Research Program of Chinese Academy of Sciences (Grant No. XDA0470102).

REFERENCES

[1] T. Andreussi, E. Ferrato, V. Giannetti, *Journal of Electric Propulsion,* 1:31, 2022.
[2] Tisaev M, Ferrato E, Giannetti V, et al., Acta Astronautica, 191: 374-393, 2022.
[3] C.Yang, Y.Hu, Journal of Astronautics, 43(2):232, 2022.

Coarse-grain modelling of a hypersonic expanding flow

C. Xie[1,a)], R. J. Gollan,[1], N. N. Gibbons[1] and C. M. Jacobs[1]

[1]*The University of Queensland, St Lucia, Queensland 4072, Australia*

[a)]Corresponding author: caiyu.xie@student.uq.edu.au

As space exploration advances, reentry into the atmosphere of the Earth is often part of the mission if samples or crew need to be returned. Thermal protection system (TPS) is imperative to protect the spacecraft from being damaged by heat during entry. Although the heating of the front body of the reentry capsule can be accurately estimated, the radiation at the expanding region at the backshell still has large uncertainties. Therefore, backshell designs rely on large safety margins [1–3]. A safety factor of 3.5 was applied for the backshell TPS of Stardust [2]. One of the reasons of the inaccuracies in backshell radiation is the uncertainty in the estimation of species population in the flow at the expanding region in nonequilibrium simulations.

Thermal nonequilibrium is usually simulated by assuming Boltzmann distribution at different temperatures for different energy modes. However, under strong nonequilibrium conditions, energy levels can deviate from Boltzmann distribution. At these conditions, state-to-state (StS) simulations remove the Boltzmann distribution constraint and the population of each energy level is tracked individually.

The high accuracy in StS simulations is achieved with high computational costs, therefore, it is not widely used in nonequilibrium modelling. The costs can be alleviated by grouping the individual energy levels into macroscopic states, so a smaller number of states need to be tracked. This work compares two methods [4, 5] for grouping microscopic levels into macroscopic states by applying them to an experimental test case of post shock expanding flow over a wedge done in the X2 expansion tube facility at The University of Queensland.

REFERENCES

[1] F. Milos, *Journal of Spacecraft and Rockets* **34**, 705–713 (1997).
[2] C. Johnston, *Journal of Spacecraft and Rockets* 1–9 (2025).
[3] K. Edquist, A. Dyakonov, M. Wright, C. Tang, 41*st AIAA Thermophysics Conference* (2009).
[4] M. Panesi, A. Lani, *Physics of Fluids* **25**, 057101 (2013).
[5] Y. Liu, M. Panesi, A. Sahai, M. Vinokur, *The Journal of Chemical Physics* **142**, 134109 (2015).

Ionosphere-Rocket Exhaust Plume Interactions: A Hybrid CFD-DSMC Study

M. Arham[1,a)], T. Lafleur,[1], D. J. Petty[1] and G. W. Bowden[1]

[1]*School of Engineering and Technology, University of New South Wales Canberra, Campbell, ACT, Australia*

[a)]Corresponding author: muhammad.arham@unsw.edu.au

At high altitudes, exhaust plumes from launch vehicles expand to large dimensions and perturb the ionosphere through collisions and chemical reactions. Gases in the plume experience various flow regimes, moving from a highly collisional continuum zone near the nozzle to an intermediate transitional zone and then a collisionless free expansion zone. Therefore, a steady-state axisymmetric CFD-DSMC hybrid approach [1, 2] is used to capture relevant physics. For the first zone, CFD (Computational Fluid Dynamics), the Navier-Stokes equations are solved using a finite volume method over a specific domain near the nozzle exit. A constant collision frequency surface computed from the CFD solution becomes the inflow boundary for the DSMC simulation which covers the second and third zones (intermediate and collisionless). DSMC (Direct Simulation Monte Carlo) is used to simulate this region with a particle-based approach assuming a variable soft sphere collision model. This simulation is conducted using the SPARTA code (Stochastic PArallel Rarefied-gas Time accurate Analyzer). Inflow of neutral and ion species from thermosphere [3] and ionosphere [4] is included in the DSMC simulation. Dissociative recombination and charge exchange reactions are included. Steady-state plume expansion and shock formation are studied and verified against analytical results. Ionosphere-plume interactions lead to an increase in plasma concentration ahead of the plume (termed the snow-plough effect) resulting in a sharp percentage change near the bow shock. However, chemical reactions significantly decrease the concentration of charged particles in the ionosphere where mixing with exhaust plume gases occurs. That results in a change in the number of electrons passing through a control surface with distance downstream of the nozzle.

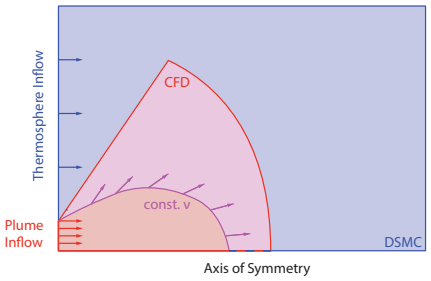


Fig. 1. Schematic diagram of the overlapping domains of the CFD and DSMC solutions for the exhaust plume flow.

REFERENCES

[1] G. W. Bowden, L. Pollock, M. Brown, *Proceedings of the 24th Australasian Fluid Mechanics Conference* (Australasian Fluid Mechanics Society, Canberra, Australia, 2024).

[2] G. W. Bowden, L. Pollock, M. Brown, *Proceedings of the 23rd Australian Space Research Conference* (National Space Society of Australia, Sydney, Australia, 2024), 77–86.

[3] J. T. Emmert, D. P. Drob, J. M. Picone, D. E. Siskind, M. Jones Jr., M. G. Mlynczak *et al.*, *Earth and Space Science,* **7**, e2020EA001321 (2020).

[4] D. Bilitza, V. Truhlik, O. Yoshihara, M. B. Moldwin, *Ann. Geophys.* **67**, SA443 (2024).

Magnetohydrodynamic Flow Control during LEO Re-entry with Realistic Magnetic Field and Capsule Geometry

L. R. Newlands[1,a)], V. Wheatley,[1] and D. E. Gildfind[1]

[1]*The University of Queensland, Brisbane, Queensland 4072, Australia*

[a)]Corresponding author: l.newlands@student.uq.edu.au

Magnetohydrodynamic (MHD) flow control utilises an applied magnetic field to manipulate high-speed plasma flows, enabling vehicle drag alteration and heat-transfer mitigation. This paper presents selected results from a preliminary computational study to investigate the feasibility of an MHD aerobraking experiment during Low Earth Orbit (LEO) re-entry [1]. The capsule geometry was based on the Kentucky Re-entry Universal Payload System (KRUPS) [2]. It was then assumed that a spherical permanent magnet was incorporated into the capsule, with several magnet radii investigated. The numerical simulations were conducted with The University of Queensland's compressible flow solver, Eilmer [3, 4]. The flow was modelled using the axisymmetric, steady-state, viscous, reacting Reynolds-Averaged Navier–Stokes equations with low magnetic Reynolds number MHD source terms and solved using a Newton-Krylov method. The results indicate that MHD flow effects are sensitive to the relative configuration of the applied magnetic field with respect to the capsule geometry. The surface-integrated heat transfer was reduced for all magnet configurations, with increasing magnet radius producing diminishing returns in heat mitigation. In contrast, the total drag response was non-monotonic, with the largest magnet achieving a substantial drag enhancement, whereas the smallest magnet produced a modest drag reduction while retaining the majority of the heat-mitigation benefit. These findings demonstrate the viability of MHD aerobraking technology, highlight the broader potential of MHD flow control in high-speed aerodynamics, and indicate that effective implementation requires careful configuration to achieve the desired aerodynamic and thermal response for a given capsule geometry and scale.

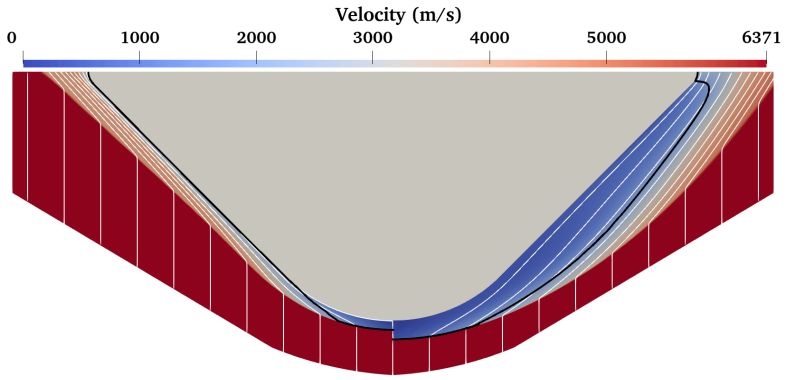


Fig. 1. Velocity field without (left) and with (right) a 4 T spherical magnetic field. Flow streamlines are visualised in white and the sonic line in black. [1]

ACKNOWLEDGEMENTS

The authors wish to thank the Eilmer development team at The University of Queensland for the development and provision of the solver used in this study.

REFERENCES

[1] L. R. Newlands, *Feasibility of an MHD Aerobraking Re-entry Experiment from the International Space Station* (Honours thesis, The University of Queensland, 2025).

[2] J. M. Cooper, J. K. Stieha, A. M. Fowler, N. A. Wright, A. Martin, *AIAA SciTech Forum (54th AIAA Aerospace Sciences Meeting)* (American Institute of Aeronautics and Astronautics, San Diego, 2016).

[3] N. N. Gibbons, K. A. Damm, P. A. Jacobs, R. J. Gollan, *Computer Physics Communications* **282**, 108551 (2023).

[4] A. Lefevre, D. Gildfind, R. Gollan, P. Jacobs, T. McIntyre, C. M. James, *AIAA SciTech Forum* (American Institute of Aeronautics and Astronautics, San Diego, 2022).

Extension of unified gas-kinetic wave-particle method to the gas mixture flow with an elementary chemical reaction

Junzhe Cao[1,a)], Yufeng Wei[1], Wenpei Long[1], Chengwen Zhong[2] and Kun Xu[1,3,4]

[1]*Department of Mathematics, Hong Kong University of Science and Technology, Hong Kong, China.*
[2]*School of Aeronautics, Northwestern Polytechnical University, 710072, Xi'an, Shaanxi, China.*
[3]*Department of Mechanical and Aerospace Engineering, Hong Kong University of Science and Technology, Hong Kong, China.*
[4]*HKUST Shenzhen Research Institute, 518057, Shenzhen, China.*

[a)]Corresponding author: jcaobb@connect.ust.hk

The unified gas-kinetic wave-particle (UGKWP) method provides significant advantages in multiscale flow from continuum to rarefied regime [1, 2]. By taking advantages of the integral solution of gas kinetic model, the mesh size is considered in the flux construction, achieving the direct modeling of physical laws in the discretized space. In the rarefied flow regime, the nonequilibrium phenomenon is evolved by the transport and relaxation of particles, making the UGKWP a Boltzmann solver. In the continuum flow regime, the near-equilibrium distribution function is represented by macroscopic variables as hydrodynamic wave, and it returns to the gas-kinetic scheme (GKS), which is a Navier-Stokes solver, thus overcoming the limitations imposed by molecular mean free path and mean collision time. The UGKWP method has been developed for a variety of multiscale physics, such as the thermal nonequilibrium flow [3], plasma transport [4], radiation transport [5], and turbulence [6]. Benefiting from the flexible and adaptive particles, the UGKWP method has advantages in high-speed flow [7] and multiphysics simulation. In this study, it is extended to gas mixture flow with an elementary chemical reaction. The kinetic model for gas mixture proposed by Todorova [8] is used, with accurate recovery of transport coefficients. The chemical reaction is split outside as a source term. An elementary chemical reaction, Zeldovich reaction, is preliminarily studied using the classical Arrhenius equation, whose macroscopic influence is linearly projected to the microscopic particles. Typical multiscale flows, such as the hypersonic cylinder flow, are simulated, and the results match well with those obtained from the DSMC method.

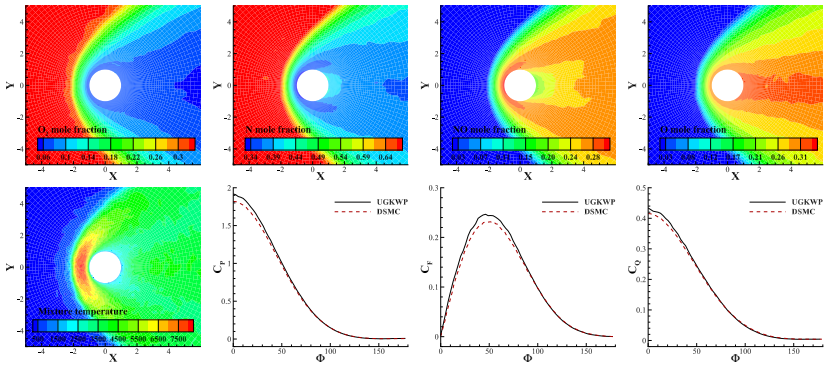


Fig. 1. Simulate the hypersonic cylinder flow with chemical reaction $O_2 + N \Leftrightarrow NO + O$ **(**$Ma = 9$**,** $Kn = 0.1$**).**

ACKNOWLEDGEMENTS

Current research is supported by National Key R&D Program of China (Grant Nos. 2022YFA1004500), National Natural Science Foundation of China (12172316, 92371107), Hong Kong research grant council (16301222, 16208324).

REFERENCES

[1] C. Liu, Y. Zhu, K. Xu, *Journal of Computational Physics* **401**, 108977 (2020).
[2] Y. Zhu, C. Liu, C. Zhong, K. Xu, *Physics of Fluids* **31**, 067105 (2019).
[3] Y. Wei, Y. Zhu, K. Xu, *Journal of Computational Physics* **497**, 112610 (2024).
[4] Z. Pu, K. Xu, *Journal of Computational Physics* 113918 (2025).
[5] X. Yang, Y. Zhu, C. Liu, K. Xu, *Journal of Computational Physics* **522**, 113587 (2025).
[6] X. Yang, K. Xu, *Physics of Fluids* **37**, 101706 (2025).
[7] W. Long, Y. Wei, K. Xu, *AIAA Journal* **62**, 1411–1433 (2024).
[8] B. N. Todorova, R. Steijl, *European Journal of Mechanics / B Fluids* **76**, 390–402 (2019).

Alternative Internal Structures of Turbomolecular Pumps Using Numerical Analysis of Rarefied Gas

H. Sugimoto[1,a)], S. Otani,[1] and M. Ito[1]

[1] *Department of Aeronautics and Astronautics, Kyoto University, Kyoto 615-8540, Japan*

[a)] Corresponding author: sugimoto.hiroshi.7s@kyoto-u.ac.jp

This study shows that the performance of conventional turbomolecular pumps (TMPs) with thin blades can be achieved with mechanically robust thick rotors through drag-pump effects revealed by rarefied gas simulations. The simulations employ two-dimensional models of single- or double-stage rotor-stator pairs placed between two tanks. Figure 1 shows the computational model of a conventional TMP. Red areas indicate the rotor blades moving with speed v_R in X_1 direction, and black lines indicate the stator blades. As illustrated in the figure, the rotor may have a finite thickness. The motion of the rotor induces the mass flux Q [1, 2], which generates a pressure ratio $p_r = \overline{p_H}/\overline{p_L}$ between the two tanks when the flow is blocked by the impermeable walls (indicated by blue lines). By repeating the simulations for various wall sizes, we obtain the model's performance curve, $p_r(Q)$. We employ the spherical design[3] for molecular velocity grids and our traveling finite-volume method[4] to compute the time evolution based on the BGK equation. Figure 2 shows the performance curve for several blade configurations. Black symbols correspond to the conventional thin blades ($d = 0$). Blades with larger θ_* produce larger Q, while those with smaller θ_* yield larger p_r. Model-D replaces rotor blades with holes, where the rotor thickness d induces a *drag pump effect*; the performance depends only weakly on d, despite the reduced conductance of the thick rotor. The drag effect can be accumulated by synchronizing the phase in model-PS. In the hybrid model, model-H in Fig. 3, a single-shape robust rotor yields comparable mass flow and pressure ratio to those of the conventional blades. The effects of the Knudsen number Kn and rotor speed v_R are also discussed.

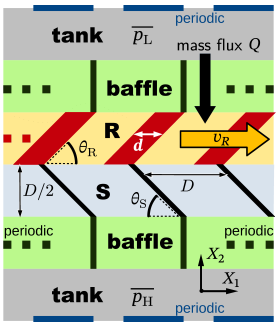


Fig. 1 An example of the computational model of TMP. The blade-pair area is $D \times D$.

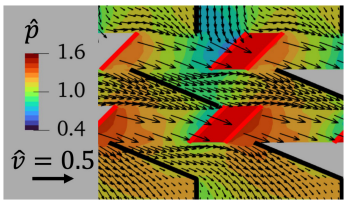


Fig. 3 Flow velocity and pressure field inside the TMP model-H. Kn = 1, $v_R/c_0 = 0.5$.

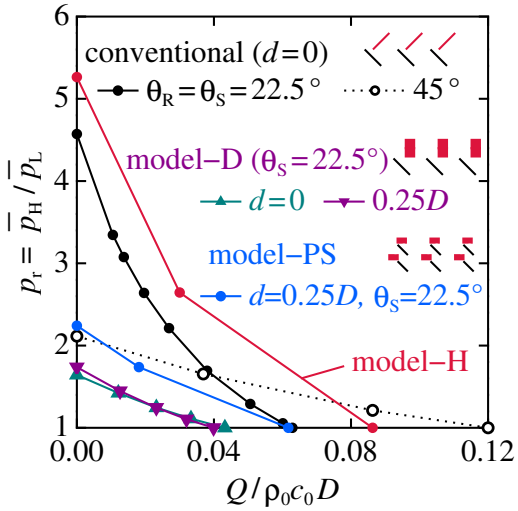


Fig. 2 Performance curves $p_r(Q)$ for thick rotor model-PS and H compared with the conventional model. The blade area is kept constant at $D \times D$ for all cases. Kn = 1, $v_R/c_0 = 0.5$ (c_0**: most probable molecular speed,** ρ_0**: average density of the gas).**

References

[1] F. Sharipov, *Journal of Vacuum Science & Technology A* **28**, 1312–1315 (2010).
[2] H. Sugimoto, A. Miki, S. Sugimoto, *Rarefied Gas Dynamics*, edited by M. T. M. Grabe, G. Oblapenko (Springer, Cham, 2026) in printing.
[3] R. S. Womersley, *Contemporary Computational Mathematics - A Celebration of the 80th Birthday of Ian Sloan*, edited by M. T. M. Grabe, G. Oblapenko (Springer, 2018), 1243–1285.
[4] R. Imazu, H. Sugimoto, M. Ito, *Rarefied Gas Dynamics*, edited by M. T. M. Grabe, G. Oblapenko (Springer, Cham, 2026) in printing.

Experimental Demonstration of Radiometric Force in a Crookes Radiometer with Isothermal Vanes

Y. Takami[1] and **H. Sugimoto**[1,a)]

[1]*Department of Aeronautics and Astronautics, Kyoto University, Kyoto 615-8540, Japan*

[a)]Corresponding author: sugimoto.hiroshi.7s@kyoto-u.ac.jp

The Crookes radiometer is an experimental apparatus that consists of a glass container enclosing low-pressure gas and a vaned wheel whose vanes are painted black on one side.[1] When exposed to light, a *radiometric force* arises, causing the wheel to rotate. Many scientists have investigated this force [2] and attributed it to thermal transpiration induced by the temperature difference between the painted side, which absorbs light, and the bare side, which reflects it. However, the existence of such a temperature difference has not been experimentally verified. To date, only one study[3] has directly measured surface temperature, and its vane structure differs from that of radiometers.

The lack of experimental evidence led to the idea that the temperature of such thin vanes would be uniform[4] according to Fourier's law of heat conduction. A uniform vane temperature would contradict the conventional explanation; nevertheless, recent studies suggest that the wheel with isothermal vanes still rotates. Chen et al.[5] demonstrated that an aluminum wheel with curved vanes rotates, and numerical work shows that, for planar vanes, a difference in accommodation coefficients between the two sides induces thermal transpiration flows.[4, 6]

This study experimentally investigates the radiometric force arising from differences in accommodation coefficients between the two sides of planar vanes. First, we measured the surface temperatures of two types of vanes: a conventional mica vane and a thin-glass vane, with one side painted black. Type-K thermocouples are attached to both sides. The vane is placed in a glass bell jar filled with helium and irradiated from both sides by two 500 W halogen lamps, as shown in Fig. 1(a). The temperature differences ΔT between the painted and bare sides for various gas pressures are plotted in Fig. 1(b) for the mica vane and in Fig. 1(c) for the glass vane. As shown in the figure, the measurable ΔT appears only for mica vanes. We will discuss the reason for the difference based on a simple thermal balance calculation.

These results enable the construction of a radiometer with nearly isothermal glass vanes, because the accommodation coefficient of helium on glass is 0.2 – 0.3[7], which is expected to be much smaller than that on a rough painted surface. Figure 2 shows the two types of radiometers with isothermal vanes. One side is painted in type-A, and both sides are painted in type-B. We have prepared two samples of each type. When illuminated in helium at 2 Pa, two type-A samples rotate at 487 and 418 rpm, respectively, from the painted side to the bare side, consistent with the direction of the thermal transpiration flow. In contrast, one of the type-B samples does not rotate, and the other type-B sample shows quite slow rotation (23 rpm). Therefore, the rapid rotation observed in type-A is attributed to thermal transpiration induced by the difference in surface treatment.

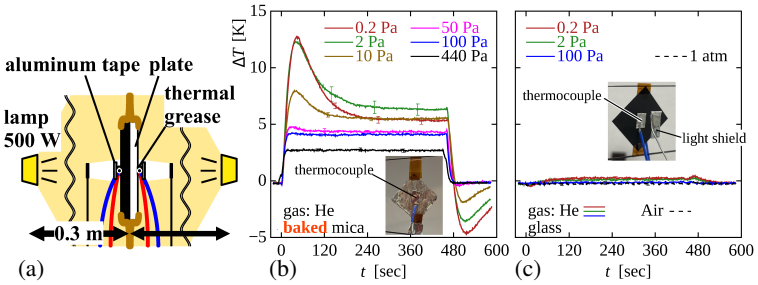


Fig. 1 Temperature difference between the painted and bare sides. (a) Baked mica vane, (b) glass vane.

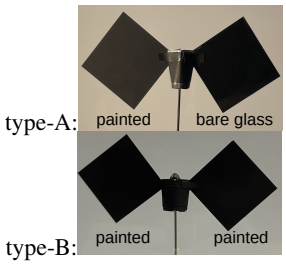


Fig. 2 Radiometer with isothermal vanes. Type-A: one side painted; Type-B: both sides painted.

References

[1] W. Crookes, *Philosophical Transactions of the Royal Society of London* 501–52712 (1874).
[2] A. Ketsdever, N. Gimelshein, S. Gimelshein, N. Selden, *Vacuum* **86**, 1644–1662 (2012).
[3] W. Gerlach, W. Schütz, *Zeitschrift für Physik* **77**, 785–800 (1932).
[4] K. Denpoh, *Journal of the Vacuum Society of Japan* **60**, 471–474 (2017).
[5] G. Chen, M. Wu, Y. Li, *Frontiers of Physics* **20**, 012201– (2025).
[6] F. Sharipov, B. C. Schafer, *Phys. Rev. Appl.* **24**, 044050Oct (2025).
[7] H. Yamaguchi, T. Imai, T. Iwai, A. Kondo, Y. Matsuda, T. Niimi, *Journal of Vacuum Science & Technology A* **32**, 06160211 (2014).

Numerical assessment of parietal accommodation at hypersonic rarefied flow conditions

B. Carda[1,2,a)], V. Lago,[2] and D. Toussaint[1]

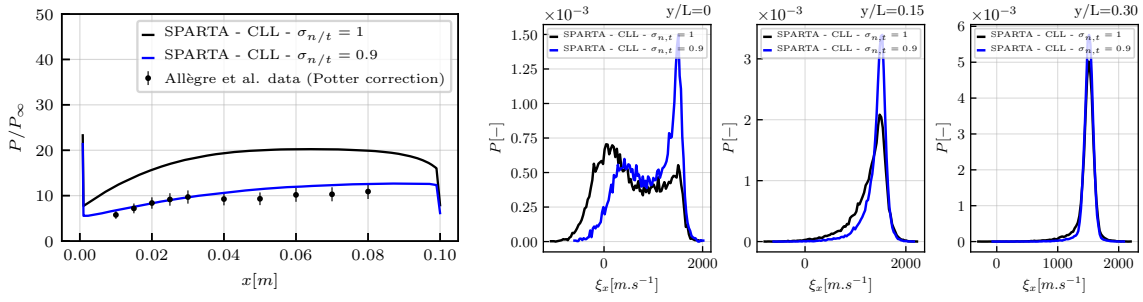
[1]*CEA-CESTA, 15 av. des Sablières - CS 60001 33116 Le Barp Cedex, France*
[2]*CNRS, ICARE, UPR 3021, 1c av. de la Recherche Scientifique, CS 50060, F-45071, Orléans cedex 2, France*

[a)]Corresponding author: beatriz.carda@cea.fr

During an atmospheric re-entry, a vehicle crosses at high velocity different layers of varying density and temperature. Those variations lead to different rarefaction regimes depending on the altitude, which affects the aerodynamic forces and heat transfer applied on the vehicle. In a previous work [1], the authors proposed a bridge function to assess the heat flux undergone by a sharp flat plate from hypersonic continuous to free-molecular regimes. This model was built using experimental and numerical data and assuming diffuse accommodation at the wall. This work is a first step to get rid of this limitation. The purpose of this work is therefore to conduct a numerical study aiming at identifying the suitable accommodation coefficients in different rarefaction regimes. Detailed knowledge of the accommodation will then be used to enhance the accuracy of the heat transfer model.

To do so, a numerical parametric study is performed to assess the wall accommodation conditions enabling the best agreement between simulations results and reference experimental data. The experimental campaign of Lengrand *et al.* [2] is used as reference: wall pressure, heat transfer and flow density profiles were measured over a beveled flat plate within the MARHy wind tunnel at three hypersonic rarefied flow conditions (Mach number of 20, Knudsen numbers of 7×10^{-3}, 2×10^{-3} and 2×10^{-4}). The numerical simulations are carried out using the *K* solver of CEA, which solves the ES-BGK model [3] using a discrete velocity approach [4] and the open-source SPARTA DSMC (Direct Simulation Monte Carlo) solver, which mimics the Boltzmann equation [5].

The 2D numerical simulations were first performed assuming spatially-constant inflow conditions. Partial parietal accommodation enabled satisfactory agreement between experimental and numerical wall quantities, namely wall pressure and heat transfer. However, the density field was not correctly assessed for accommodation coefficients below unity. One set of coefficients would therefore not seem to enable to replicate both wall and flowfield quantities. The discrepancies observed between experimental and numerical density values are suspected to result from density gradients at the nozzle outlet. A simulation of the flow within the nozzle is thus in progress to take into account this phenomenon. The velocity and density profiles obtained at the nozzle outlet will then constitute the inflow conditions for improved flat plate calculations. In addition, the impact of partial accommodation on the flow above the plate was studied. The velocity distributions in the longitudinal and transverse directions for several accommodation coefficients were calculated. The influence of wall conditions is discernable across the entire thickness of the shock layer (fig. 1b). Lastly, results from a new experimental campaign within the MARHy windtunnel, aiming at complementing Lengrand's data to better understand parietal accommodation, will also be discussed in the presentation.



(a) (b)

Fig. 1. : Normalized wall pressure (a) and velocity distribution along *y* (b) obtained with different accommodation conditions at Mach 20.2 - 0.067Pa - Kn = 7×10^{-3}.

REFERENCES

[1] Proceedings of the 3rd International Conference on Flight vehicles, Aerothermodynamics and Re-entry (FAR 2025) (European Space Agency, 2025).
[2] J. Lengrand, J. Allegre, A. Chpoun, M. Raffin, Progress in astronautics and aeronautics **160**, 276–276 (1994).
[3] L. H. Holway, Jr., Rarefied Gas Dynamics, Volume 1 (1965) 193.
[4] C. Baranger, J. Claudel, N. Hérouard, L. Mieussens, Journal of Computational Physics **257**, 572–593January (2014).
[5] S. J. Plimpton, S. G. Moore, A. Borner, A. K. Stagg, T. P. Koehler, J. R. Torczynski, M. A. Gallis, Physics of Fluids **31**, 08610108 (2019).

Rotation-Based Dimensional Reduction for Nonlinear Moment Closures in Multidimensional Kinetic Systems

Eda Yilmaz[1,a)] and Manuel Torrilhon[1]

[1]*Applied and Computational Mathematics (ACoM), RWTH Aachen University, Germany*

[a)]yilmaz@acom.rwth-aachen.de

Rarefied gas flows often operate beyond the validity range of classical fluid models, since the Navier–Stokes–Fourier equations fail to accurately describe strong non-equilibrium effects. A fundamental description is provided by the Boltzmann equation, which governs the evolution of the particle distribution function in phase space [1]. However, its direct numerical treatment remains computationally prohibitive due to the high dimensionality of the velocity variable and the nonlinear structure of the collision operator.

Moment methods provide a systematic reduction by projecting the kinetic equation onto a finite-dimensional space spanned by velocity monomials. The resulting moment system forms an open hierarchy, as the evolution of moments of order n depends on those of order $n + 1$. Closure relations are therefore required to obtain a finite system. Classical approaches, such as Grad's Hermite expansion [1] and entropy-based closures [2, 3], exhibit favorable properties in one-dimensional settings but encounter difficulties in multidimensional or far-from-equilibrium regimes. In particular, polynomial closures may lose hyperbolicity, while entropy-based methods, although structurally robust, require the solution of costly optimization problems.

Recently, a Gramian closure was proposed for one-dimensional moment systems [5]. The method constructs orthogonal polynomials from the known lower-order moments via the Gram matrix, whose entries consist of weighted inner products of velocity monomials. This framework yields explicit expressions for higher-order moments without reconstructing the underlying distribution function. Moreover, extended formulations allow separate treatment of even and odd orders, enabling control of structural properties such as hyperbolicity and equilibrium consistency.

Extending this methodology to three-dimensional moment tensors presents significant challenges. The number of independent tensor components grows rapidly with moment order, and a direct multidimensional Gramian construction becomes algebraically intricate. In this work, we propose a rotation-based dimensional reduction strategy. The central idea is to exploit rotational invariance of the kinetic framework: the multidimensional moment tensor is transformed under a set of rotations, and for each orientation a one-dimensional projection along a chosen axis is obtained. The 1D Gramian closure is then applied independently to these projected systems. By collecting the closure outputs for sufficiently many rotations, we obtain a linear reconstruction problem whose solution yields the full three-dimensional higher-order moment tensor.

This approach allows the explicit and computationally efficient reconstruction of multidimensional higher-order moments while preserving essential tensorial properties such as symmetry and trace invariance. The proposed framework demonstrates how a nonlinear 1D closure technique can be systematically lifted to multidimensional systems, providing a practical and structurally consistent tool for rarefied gas modeling.

ACKNOWLEDGEMENTS

This research was supported by the German Research Foundation within the research unit DFG-FOR5409.

REFERENCES

[1] H. Grad, Commun. Pure Appl. Math. 2(4):331–407, 1949.
[2] N. Böhmer and M. Torrilhon, J. Comput. Phys. 401:108992, 2020.
[3] C. D. Levermore, Transport Theory Stat. Phys. 26(4–5):591–606, 1997.
[4] M. Torrilhon, Annu. Rev. Fluid Mech. 48:429–458, 2016.
[5] E. Yilmaz, G. Oblapenko, M. Torrilhon, arXiv:2407.05894, 2024.
[6] R. O. Fox, F. Laurent, SIAM J. Appl. Math. 82:750–771, 2022.

Analysis of Fast-Converging and Asymptotic-Preserving DSMC Boosted by GSIS Intermittently

B. Hu[1,a)], L. Luo[1], K. Wang[1] and L. Wu[1]

[1]*Southern University of Science and Technology, China*

[a)]Corresponding author: wul@sustech.edu.cn

The direct simulation Monte Carlo (DSMC) method is a widely used stochastic approach for rarefied gas flows. However, its computational efficiency deteriorates severely in near-continuum and multiscale regimes, as the time step and cell size must be smaller than the mean free path and collision time, leading to a large number of particles and iterations when the Knudsen number becomes small. To overcome this limitation, the direct intermittent general synthetic iteration (DIG) scheme has been recently proposed to enable the DSMC method to converge rapidly and accurately to steady-state solutions. The key process of DIG is the alternative solving of the macroscopic synthetic equations and the mesoscopic equation via DSMC. The time-averaged macroscopic properties and high-order constitutive relations extracted from the DSMC simulations are utilized to solve the synthetic equations. The resulting updated solution is subsequently fed back into DSMC to modify the particle velocities, thereby reducing unnecessary iterations and accelerating the flow field toward a steady state. In our work, we investigate the fast-converging and asymptotic-preserving (FC-AP) properties of DIG through both theoretical analysis and numerical validation. Owing to the analytical intractability of the Boltzmann equation, the theoretical analysis is conducted using the linearized BGK model. Fourier stability analysis demonstrates the FC property that in the near-continuum regime, the error is reduced by at least a factor of five after a single DIG cycle. Moreover, the Chapman-Enskog expansion shows that the AP of DIG enables the Navier-Stokes limit to be accurately recovered even when the cell size is of order O(1). The accuracy and efficiency of DIG are further validated by DSMC simulations of Poiseuille flow and hypersonic flow over a cylinder. The results indicate that DIG significantly reduces the number of iterations and spatial cells required for convergence, leading to a substantial reduction in computational cost. For example, at Kn = 0.01, DIG achieves nearly two orders of magnitude fast than DSMC, with even greater performance gains at smaller Knudsen numbers, which demonstrates the strong potential of DIG for engineering applications in near-continuum and multiscale gas flows.

Machine Learning-Based Gas-Surface Scattering Model for Direct Simulation Monte Carlo Simulations in Very Low Earth Orbit

M. Schütte[1,a)], S. Fasoulas[1] and M. Pfeiffer[1]

[1] *University of Stuttgart, Institute of Space Systems, Pfaffenwaldring 29, 70569 Stuttgart, Germany.*

[a)] Corresponding author: schuettem@irs.uni-stuttgart.de

Very low Earth orbit (VLEO), defined as orbit altitudes below 450 km, has become increasingly attractive for satellite missions. The benefits of VLEO include reduced launch costs and the rapid natural removal of debris due to enhanced atmospheric drag at these altitudes. However, this same atmospheric drag significantly reduces the operational lifespan of satellites, necessitating the use of propulsion systems to maintain orbit [1, 2].

Given the free molecular flow regime in VLEO, the Direct Simulation Monte Carlo (DSMC) [3] method is required to model gas-surface interactions (GSI) on satellites. Nonetheless, its accuracy is highly constraint by the limited fidelity of existing GSI models, which often rely on constant accommodation coefficients and assume independent scattering in the normal and tangential directions. Incorporating a more physically accurate model would significantly improve mission design and propellant requirements, potentially extending operational lifetimes and lowering costs. In addition, harnessing aerodynamic lift for altitude and orbit control can further reduce dependence on thrusters and fuel.

On the other hand, molecular dynamics (MD) simulations enable highly accurate modeling of gas–surface interactions at the microscopic level, offering detailed insight into the underlying physical mechanisms. However, their substantial computational cost makes it infeasible to apply MD directly to simulations at the scale of an entire satellite. We introduce an advanced modeling strategy that uses MD simulation data to train a machine learning (ML) model, like a normalizing flow (Fig. 1) or a conditional variational autoencoder (Fig. 2), resulting in a high-fidelity scattering kernel. This kernel is directly embedded into DSMC simulations, substantially enhancing their accuracy. By converting atomistic interaction data into a data-driven boundary condition, the proposed hybrid framework connects microscopic surface physics with macroscopic aerodynamic behavior.

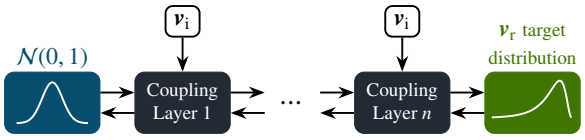


Fig. 1. Normalizing flow.

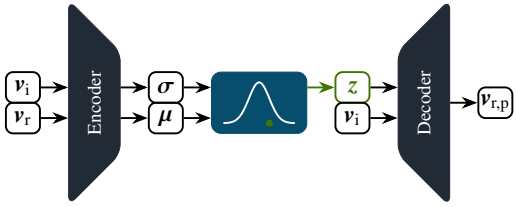


Fig. 2. Conditional variational autoencoder.

ACKNOWLEDGEMENTS

This work is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 516238647 – SFB 1667 (ATLAS - Advancing Technologies of Low-Altitude Satellites).

REFERENCES

[1] N. Crisp *et al.*, *Progress in Aerospace Sciences* **117**, 1–18 (2020).
[2] J. Virgili-Llop *et al.*, *Proc. of the Reinventing Space Conference* (London, UK, 2014).
[3] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Oxford University Press, Oxford, UK, 1994).

Abstract 93

DSMC-Based Analysis of Gas Flow Behavior in Particle Exhaust Systems of Fusion Reactors

F. Litovoli[a)], C. Tantos, H. Strobel

Karlsruhe Institute of Technology, 76344, Eggenstein-Leopoldshafen, Germany.

[a)] Corresponding author: foteini.litovoli@kit.edu

The ongoing global energy crisis, driven by increasing energy demand, climate change, and the limitations of conventional energy sources, has highlighted the urgent need for reliable, sustainable, and low-carbon alternatives. In this context, nuclear fusion has emerged as a promising long-term option, offering the potential for abundant energy with minimal environmental impact. Achieving reliable and efficient fusion power, however, requires the development of robust reactor systems capable of handling extreme thermal and particle loads. The particle exhaust system, as one of the main reactor subsystems, is critical to the performance and long-term viability of fusion reactors, directly governing reaction efficiency and sustainability. At the heart of this system, the divertor is engineered to safely extract heat and remove impurities generated during fusion. Modelling the divertor region, however, remains a great challenge due to its intricate three-dimensional geometry and the complex behaviour of neutral gas flows, which span a wide range of rarefaction and collisionality.

In the present work, advanced numerical simulations of the particle exhaust system of the Demonstration Power Plant (DEMO) fusion reactor are presented, with particular emphasis on the divertor region. The Direct Simulation Monte Carlo (DSMC) method is employed to accurately describe the gas behaviour across the full range of collisionality relevant to divertor conditions [1-3]. The simulations are performed under representative plasma boundary conditions, enabling a detailed analysis of neutral particle transport, pumping efficiency, and leakage phenomena within the divertor volume. Multiple aspects of the divertor geometry are examined, the influence of key physical and geometrical effects is assessed, and the role of three-dimensional leakage paths is investigated. The results provide insights into neutral gas behaviour in complex fusion geometries and contribute to the ongoing optimization of the DEMO and other future fusion reactors.

REFERENCES

[1] C. Tantos, S. Varoutis, C. Day, *J. Vac. Sci. Technol. B.*, **38**, pp. 064201 (2020).
[2] C. Tantos, S. Varoutis, V. Hauer, C. Day, P. Innocente, *Nucl. Fusion*, **64**, pp 016019 (2023).
[3] C. Tantos, H. Strobel, V. Hauer, C. Day, T. Giegerich, P. Innocente, *Fusion Eng. Des.*, **215**, pp. 115021 (2025).

Abstract 94

Modelling rarefied gas mixture flows using various kinetic approaches

T. Basdanis[1,a)], C. Tantos[1], T. Teichmann[2]

[1] *Institute for Technical Physics, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany*
[2] *Kyoto Fusioneering Europe GmbH, 76227 Karlsruhe, Germany*

[a)] Corresponding author: athanasios.basdanis@kit.edu

Rarefied gas flows play a central role in the design and optimization of modern technologies such as MEMS, micro-propulsion systems, vacuum devices, and fusion reactors, where the molecular mean free path becomes comparable to characteristic length scales. In these regimes, the continuum description loses its validity and a kinetic description based on the Boltzmann equation is required [1]. While extensive studies exist for single-gas rarefied flows in simple, uniform microchannels, systematic deterministic kinetic investigations of gas-mixture flows in non-uniform geometries commonly encountered in vacuum and micro-scale technologies remain unexplored [2].

This study investigates the behavior of binary gas-mixture flows in channels, under conditions which are relevant to microfluidic and vacuum systems. The analysis is based on the Discrete Velocity Method (DVM) [3] and the stochastic Direct Simulation Monte Carlo (DSMC) [4] method, which are employed to model both low- and high- speed flows. The research examines how key factors—such as Knudsen number, channel geometry, and gas mixture composition—affect mass flow rates, gas separation efficiency, and overall flow structure under rarefied conditions. Special emphasis is placed on understanding the transition and near free-molecular regimes, where traditional flow models begin to lose their applicability. The findings contribute to refining our understanding of gas mixture dynamics in confined geometries and provide a strong foundation for designing more efficient systems in emerging technologies, including microfluidic devices, gas separation processes, and vacuum-based applications.

REFERENCES

[1] C. Cercignani, *The Boltzmann Equation and Its Applications,* (Springer, 1988).
[2] C. Tantos, T. Teichmann, I. Sarris, C. Day, *Physics of Fluids,* 36, 012009 (2024).
[3] F. Sharipov, *Rarefied Gas Dynamics, Fundamentals for Research and Practice,* (Wiley, Hoboken, 2016).
[4] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Oxford University Press Inc., New York, 1994).

Kinetic simulations of non-equilibrium ionization and excitation in laser-induced plasma plumes

Alexey N. Volkov[1*], Michael A. Stokes[1], Tanner Tripoli[1], Michael Wolkow[1], and Zhibin Lin[2]

[1] *Department of Mechanical Engineering, University of Alabama, H.M. Comer Hall, 7th Avenue, Tuscaloosa, AL 35487, USA.*
[2] *MKS Inc., 14523 SW Millikan Way, Beaverton, Oregon 97005, USA.*

[a)] Corresponding author: avolkov1@ua.edu

In recent literature, the model of Saha-Boltzmann ionization and excitation equilibrium is routinely used to predict ionization and radiation absorption in plumes induced by irradiation of material targets with ns laser pulses. In the present work, the equilibrium ionization model (EQM) and non-equilibrium collisional-radiative model (CRM) are compared under typical conditions of ns single- and multi-pulsed laser ablation to reveal the effect of plasma non-equilibrium on radiation absorption and degree of plasma shielding. The simulations of plume expansion induced by irradiation of a copper target in vacuum or 1 atm argon background gas with Gaussian and flat-top laser pulses are performed with a hybrid computational model (Fig. 1(a)). The model includes a thermal model of the irradiated target, a model of radiation transfer, and a lumped particle direct simulation Monte Carlo (ℓDSMC) method coupled with either CRM or EQM [1,2]. The simulations show that EQM strongly underestimates the effects of ionization and radiation absorption compared to CRM (Fig. 1(b)). These results are explained by the coupling between plume expansion and the dynamics of electron temperature and ion population densities of the excited states in CRM and EQM. The ℓDSMC-CRM model is also combined with the particle-in-cell (PIC) method to account for charge separation effects. The ℓDSMC-CRM-PIC simulations predict double-layer formation resulting in stronger plume acceleration compared to the simulations without charge separation. This study indicates that the model of Saha-Boltzmann equilibrium can fail to predict radiation absorption, ionization, and the degree of plasma shielding in nanosecond laser ablation.

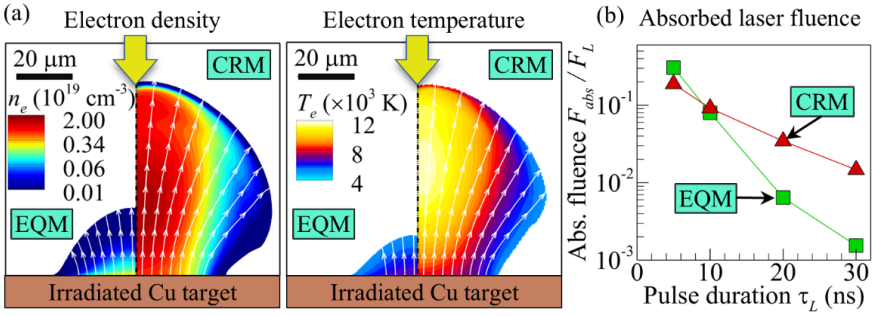


Figure 1: (a) Electron density and temperature at laser ablation of copper into 1 atm argon gas obtained with EQM and CRM for a flattop laser pulse of wavelength 266 nm, duration $\tau_L = 60$ ns, and peak fluence $F_L = 16.6$ Jcm^{-2}; (b) Fraction of peak fluence absorbed in the plume F_{abs} versus τ_L obtained with EQM (squares) and CRM (triangles) at $F_L = 8$ Jcm^{-2} [1].

ACKNOWLEDGEMENTS

This work was supported by the National Science Foundation, USA through RII-Track-1 Future Technologies and Enabling Plasma Processes project (award OIA-2148653) and MKS Instruments, Inc.

REFERENCES

[1] M.A. Stokes, A.N. Volkov, S.A. Khairallah, A.M. Rubenchik, and Z. Lin (2026, under review).
[2] M.A. Stokes, A.N. Volkov, Z. Lin, S.A. Khairallah, *J. Phys. D: Appl. Phys.* 58, 41LT01 (2025).

A Molecular Dynamics Study of Evaporation and Condensation of Atomic Clusters at a Metal Surface as well as Cluster Growth in the Vapor Phase

Alexey N. Volkov[1,a], Saeed Siahtiri[1], and Lily Stubblefield[1]

[1] Department of Mechanical Engineering, University of Alabama, 7th Avenue, Tuscaloosa, AL 35487, USA.

[a)] Corresponding author: avolkov1@ua.edu

Understanding the fundamental mechanisms of evaporation and condensation phenomena at interfaces between liquid metals and vapors is important for applications in thermal management, phase-change heat transfer, and high-temperature material processing and manufacturing, including laser ablation and laser powder bed fusion. In hydrodynamic and kinetic simulations of vapor flows, it is usually assumed that only evaporation of monomers occurs at the liquid surface, while the formation of clusters proceeds via nucleation, collisions, and growth processes in the vapor volume.

The goal of this work is to study the mechanisms of material evaporation and condensation from a liquid metal surface under conditions of normal evaporation, when the surface temperature is below the thermodynamic critical temperature, as well as cluster growth in the vapor phase. For this purpose, large-scale molecular dynamics (MD) simulations of equilibrium evaporation and condensation at the interface between liquid copper and copper vapor, as well as non-equilibrium simulation of impact of copper clusters on a liquid copper surface are performed. The embedded atom method potential is used to accurately capture metallic bonding and interatomic interactions. The simulations were conducted at temperatures ranging from 2000 K to 5500 K. To analyze the cluster content in the vapor phase and to distinguish between stable clusters and unstable atomic complexes, a special lifetime-based retrospective cluster identification algorithm is developed and used for post-processing of results of time-dependent MD simulations.

The simulations indicate that, contrary to the traditional assumption of single-atom removal during the evaporation process, emission of clusters from the liquid metal surface takes place, and the molar fraction of clusters in the evaporation flux can be as large as 30%. The content of clusters that are larger than trimers in the evaporation flux is substantially higher than the equilibrium fraction of such clusters in the vapor phase. The velocity distribution functions of evaporated monomers and clusters are nearly Maxwellian at a quasi-relaxation temperature that is smaller than the system temperature. The equilibrium evaporation coefficient is calculated and found to be significantly smaller than 1 at temperatures greater than 3000 K. The probability of condensation of monomers and dimers is calculated as a function of the impact speed, angle of incidence, and liquid surface temperatures in non-equilibrium MD simulations. The results of MD simulations are used to formulate the semi-empirical kinetic boundary conditions for evaporation and condensation of clusters at a metal surface.

In addition, the results of equilibrium MD simulation are used to determine the rates of various non-elastic collision processes between clusters in the vapor phases leading to the cluster growth or fragmentation. The results of these simulations are compared with the kinetic models of cluster growth that were suggested in the literature for simulations based on the direct simulation Monte Carlo (DSMC) method. This comparison is used to find the DSMC model parameters, such as kinetic rate coefficient for the dimer nucleation as well as sticking and evaporation probabilities of monomers, which enable matching the results of the MD and DSMC simulations. Thus, this work led to the formulation of the DSMC model of copper cluster dynamics in the vapor phase which is able to produce the results in agreement with results of the MD simulations.

ACKNOWLEDGEMENTS

This work was supported by the National Science Foundation, USA through RII-Track-1 Future Technologies and Enabling Plasma Processes project (award OIA-2148653).

Extension and application of a quantum lattice Boltzmann method to free molecular flow around a flat plate

A. Nagel[1,2,a)] and L. Basov[1,3]

[1]*German Aerospace Center (DLR), Bunsenstrasse 10, 37073 Göttingen, Germany*
[2]*University of Göttingen, Faculty of Physics, Friedrich-Hund-Platz 1, Göttingen, 37077, Germany*
[3]*Applied and Computational Mathematics, RWTH Aachen, Schinkelstrasse 2, Aachen, 52062, Germany*

[a)]Corresponding author: aaron.nagel@dlr.de

The simulation of gas flows for reentry problems can require to resolve a larger range of spatial scales in order to accurately model the physics of the flow field. In hypersonic flows, the modeling additionally requires to cover a large range in the velocity subspace of the phase space. Scale resolving methods like the Direct Simulation Monte Carlo (DSMC) method have been developed [1] but can become computationally very expensive and unfeasible. Therefore, approximation methods allowing coarser grids are used which, however, may not be sufficiently accurate.

To enable more efficient simulation methods, first approaches of a quantum lattice-gas model have been developed [2] but these model do not scale efficiently with the grid resolution [3]. Building on these quantum algorithms, promising modeling approaches using a quantum lattice Boltzmann method (QLBM) with amplitude encoding have shown to efficiently deal with very large grids and fine discretizations [4, 5]. Fine resolution of position and velocity space in the context of lattice Boltzmann methods (LBM) translate to many grid cells and a large set of velocity vectors in the LBM velocity discretization stencil, which can be encoded to scale efficiently in a qubit representation using the QLBM.

For the investigation of collisionless flows a method based on Todorova et al. [5] has been adopted and extended (cf. Fig. 1) to build upon our previous publication [6]. The streaming and boundary interaction are modeled as two independent modular blocks, where the streaming block is adapted to be performed independently of the boundary. Additionally, our quantum algorithm includes the summation of the velocity distribution functions to calculate the mass density distribution directly in the quantum simulation. In contrast to a summation by classical post processing, the quantum summation block enables further development to extract reduced data from the quantum computer. This is a key point to not having to extract the entire high dimensional quantum state vector.

In this study, a hypersonic collisionless flow around a flat plate with specular reflection is simulated using a quantum lattice Boltzmann method and compared with results using the established DSMC method for modeling rarefied flows. The quantum simulation is performed using a quantum algorithm simulator. Further approaches on how to extend the specular reflection model to a diffusive reflecting model are sketched out.

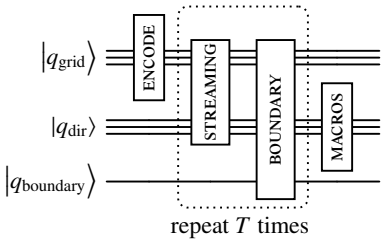


Fig. 1. Schematic QLBM simulation structure for T time steps.

ACKNOWLEDGEMENTS

This project was made possible by the DLR Quantum Computing Initiative and the Federal Ministry for Economic Affairs and Climate Action; *qci.dlr.de/projects/toquaflics*.

REFERENCES

[1] G. A. Bird, *Molecular gas dynamics and the direct simulation of gas flows* (Oxford university press, 1994).
[2] J. Yepez, *Physical Review E* **63**, 046702 (2001).
[3] M. A. Schalkers, M. Möller, *Quantum Information Processing* **23**, 20 (2024).
[4] S. Succi, F. Fillion-Gourdeau, S. Palpacelli, *EPJ Quantum Technology* **2**, 1–17 (2015).
[5] B. N. Todorova, R. Steijl, *Journal of Computational Physics* **409**, 109347 (2020).
[6] A. Nagel, J. Löwe, *Computer Physics Communications* 110040 (2026).

Accelerated Oxide Formation and Functional Degradation of Conductive Materials in Reactive, Rarefied Plasma Environments

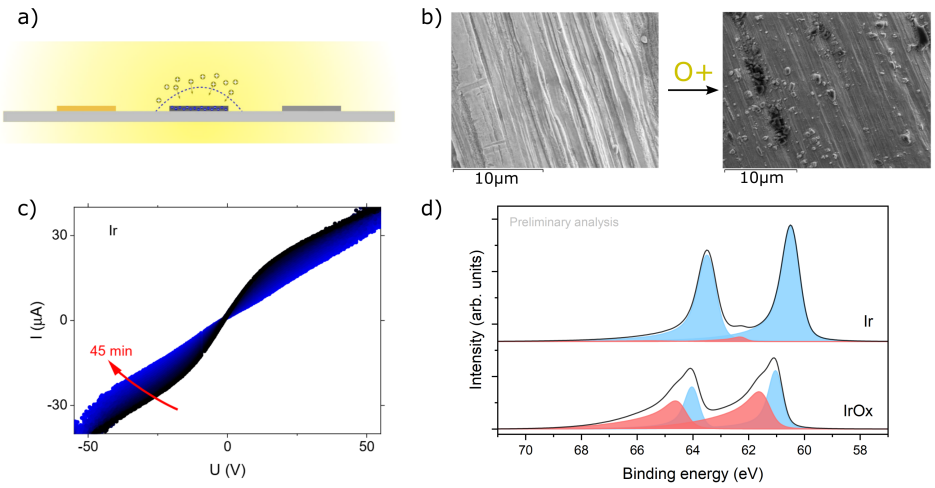
Rodrigo Sandoval Rodriguez[1,a)], Kalle Bräumer[1], Jana Zorn[1], Jan Luka Dornseifer[1], Kristof Holste,[1] and Peter J. Klar[1]

[1] *Justus Liebig University Giessen, Institute of Experimental Physics I, Heinrich Buff Ring 16, 35392 Giessen, Germany*

[a)]Corresponding author: rodrigo.ignacio.sandoval.rodriguez@physik.uni-giessen.de

Conductive materials exposed to reactive, rarefied oxygen environments experience accelerated oxide formation that can significantly degrade functional properties such as electrical conductivity. In reactive, non-equilibrium environments, oxidation kinetics are governed by the incident O and O^+ fluxes and their energy distributions. Atomic oxygen promotes rapid oxidation, while sheath-accelerated ions enhance defect generation and oxygen incorporation [1]. Together, these mechanisms are consistent with a transition from Cabrera–Mott-type self-limiting growth at nanometre scale toward diffusion-limited behaviour at larger oxide thicknesses [2].

This work examines oxide growth and functional degradation of conductive materials during exposure to reactive, rarefied oxygen plasmas in the commissioning phase of an atomic oxygen facility targeting directed, hyperthermal AO beam operation for VLEO simulation. Metals, alloys, and transparent conducting oxides are subjected to controlled plasma exposure to assess changes in surface morphology, composition, and electrical performance. The reactive oxygen environment is characterised using trace rare gases optical emission spectroscopy and actinometry to quantify electron temperature and dissociation levels during exposure. Post-exposure characterisation using scanning electron microscopy (SEM), energy-dispersive x-ray spectroscopy (EDX), and x-ray photoelectron spectroscopy (XPS) reveals material-dependent oxidation behaviour, including rapid initial passivation and self-limited oxide growth. Electrical conductivity measurements demonstrate pronounced functional degradation even after short exposure times.



Overview of oxidation and functional degradation of conductive materials. (a) Schematic of plasma-material interaction illustrating the role of sheath-accelerated O^+ ions and neutral atomic oxygen in driving surface oxidation. (b) SEM images of a tungsten surface before and after oxygen ion exposure, showing the development of oxide clusters on the surface. (c) In-situ evolution of I(U) characteristics of an iridium probe during prolonged oxygen plasma exposure, demonstrating a progressive change in electrical conductivity with exposure time. (d) XPS Ir 4f core-level spectra of metallic Ir (top) and oxidized IrO_x (bottom) after plasma exposure.

REFERENCES

[1] C. Yuan, D. Zhang, Y. Gan, *ACS Omega* **9**, 28912–28925 (2024).

[2] N. V. Alov, *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* **256**, 337–340 (2007), atomic Collisions in Solids.

Stability and Transition Investigations for an Accelerated Boundary-Layer at Mach 5 – 7.5 for the Free-Flight Measurements GAsFEx II

L. Bott[1,a)], C. Capecchi[1], C. Stemmer[1], I. Jahn[2], J. Williamson[2], M. van Hoffen[2], M. Hörschgen-Eggers[3], M. Hiepp[3], R. Kirchhartz[3] and R. Pietsch[4]

[1]*Chair of Aerodynamics and Fluid Mechanics, Technical University of Munich (TUM), München, Bavaria, Germany*
[2]*University of Southern Queensland (UniSQ), Springfield, Queensland, Australia*
[3]*Deutsches Zentrum für Luft- und Raumfahrt (DLR), Oberpfaffenhofen, Bavaria, Germany*
[4]*HyperFlight Systems, Brisbane, Queensland, Australia*

[a)]Corresponding author: lennart.bott@tum.de

We investigate laminar-turbulent transition at the ogive/conical front section of DLR's MAPHEUS 16 sounding rocket vehicle launched in November 2025 using the Direct Numerical Simulation (DNS) code NSMB (Navier-Stokes Multi-Block) [1]. The rocket reached Mach numbers up to $Ma = 7.7$ and Reynolds numbers in the order of $Re \sim 10^7$ during the hypersonic flight phase where laminar-turbulent transition is to be expected in the front section of the rocket (nose cap/cone and ogive). Free-flight pressure and temperature sensor data are gathered at specified locations along the ogive providing flight data for relevant conditions and allowing for a comparison to the numerical results. Linear stability theory (LST) for hypersonic flows [2] is employed to analyze the stability of high-resolution, laminar, two-dimensional, axisymmetric, steady base flows in the Mach-range of $Ma = 5 - 7.7$. A 4^{th} order central skew-symmetric space scheme with explicit time stepping is employed to minimize numerical dissipation, and to resolve the viscous boundary layer gradients well.
A detached bow shock develops upstream of the rocket's blunt nose leading to relevant concentrations of dissociated oxygen. Due to manufacturing inaccuracies, a chamfer with negative inclination and a backward-facing step are present between the nose tip and the ogive of the rocket. A small and stable separation bubble containing two counter-rotating vortices forms as a consequence. As the backward-facing step is located only a few centimeters downstream of the stagnation point, it is expected to be upstream of the synchronization point for fast and slow acoustic instability waves. Whether said geometric feature and position are sufficient to significantly alter the stability of the boundary-layer flow needs to be investigated [3, 4]. Flows around ogive bodies are accelerated and exhibit a negative pressure gradient, leading to more stable boundary-layer flow and delayed transition [5]. By identifying the critical frequency range using LST, a roughness element will be designed and placed at a favorable position to trigger transition in unsteady simulations [6]. Future work will be devoted to determine the influence of three-dimensional isolated roughness, discontinuities as well as roughness patches on the stability of the boundary layer extending the work of Chiapparino and Stemmer [7] for the flow over a ramp.

ACKNOWLEDGEMENTS

The authors gratefully acknowledge the Deutsche Forschungsgemeinschaft DFG (grant nb. 553275632) and the International Graduate School of Science and Engineering (project nb. P2302) for funding this project. Furthermore, they express their gratitude to the Leibniz Supercomputing Centre (www.lrz.de) and the Gauss Centre for Supercomputing e.V. (www.gauss-centre.eu) for providing computational and data resources. The authors would like to thank their project partners at UniSQ and, in particular, Mr. James Leader for his work on GAsFEx I and the sensor inserts, as well as Dr. Ray Malpress for the design and manufacturing of the fast-response thermocouples. Finally, the authors thank the DLR and especially the MAPHEUS 16 campaign team for their support.

REFERENCES

[1] Y. Hoarau, D. Pena, J. B. Vos, D. Charbonier, A. Gehri, M. Braza, T. Deloze, E. Laurendeau, *54th AIAA aerospace sciences meeting* (2016) 2056.
[2] M. L. Hudson, N. Chokani, G. V. Candler, *AIAA Journal* **35**, 958–964 (1997).
[3] G. Gong, G. Tu, B. Wan, C. Li, J. Chen, W. Hu, *Physics of Fluids* **36** (2024), 10.1063/5.0185623.
[4] J. A. Franco, S. Hein, A. Wagner, *4th International Conference on High-Speed Vehicle Science and Technology HiSST 2025* (2025), 1–10.
[5] C. Stemmer, *Turbulence and Transition in Supersonic and Hypersonic Flows* (2026), 3–34.
[6] S. Hein, A. Theiss, A. Di Giovanni, C. Stemmer, T. Schilden, W. Schroeder, P. Paredes, M. Choudhari, F. Li, E. Reshotko, *Journal of Spacecraft and Rockets* **56**, 388–404 (2019).
[7] G. Chiapparino, C. Stemmer, *International Journal of Heat and Fluid Flow* **103** (2023), 10.1016/j.ijheatfluidflow.2023.109193.

Influence of wall-temperature distribution on hypersonic boundary-layer stability

C. Capecchi[1,a)] and C. Stemmer[1]

[1]*Chair of Aerodynamics and Fluid Mechanics, Technical University of Munich (TUM), München, Bavaria, Germany*

[a)]Corresponding author: cosimo.capecchi@tum.de

Laminar-turbulent transition in hypersonic boundary-layers strongly influences aerodynamic heating, drag, and overall vehicle operability. Transition leads higher viscous drag as well as to an increased heat transfer, requiring stronger or more advanced thermal protection systems (TPS). These effects highlight the importance of understanding the transition process in hypersonic regimes. The present study specifically investigates the impact that localized wall heating on a flat plate has on the laminar-turbulent transition.

Direct Numerical Simulations (DNS) are performed using the semi-commercial solver Navier-Stokes Multi-Block (NSMB) [1], a finite-volume solver using the Message Passing Interface (MPI) protocol to parallelize the computations on structured multi-block grids. It has already been employed and validated in a variety of hypersonic flow calculations [2–4]. The 2D steady laminar base-flow simulations of the flat plate reproduce the operating conditions of the T4 shock tunnel, as in Table 1., using a 4^{th} order skew-symmetric central spatial numerical scheme in order to properly resolve the viscous boundary layer present in the flow field. The wall boundary conditions are modified to match the temperature distribution produced by a heating device developed by the Centre for Hypersonic at the University of Queensland (UQ).

The first objective of the study is to determine the position of the synchronization point by analysing the fast and slow modes behaviour via Linear Stability Theory (LST) analysis at the given experimental conditions at T4. The LST results are validated against known cases in literature as well as against unsteady DNS simulations. Once the synchronization point is obtained, we follow the approach by [5] influencing the boundary-layer stability properties by introducing augmented wall-temperature. By positioning the heating patch after the synchronization point, the boundary layer is expected to show a delayed transitioning region.

The final goal is to gain deeper insight into the transition mechanisms influenced by local wall heating comparing the numerical results to the experimental measurements obtained in the T4 hypersonic shock tunnel at UQ [6]. This side-by-side comparison is intended to evaluate, in a controlled setting, the influence of prescribed wall-temperature distributions on boundary-layer stability and the evolvement of laminar-turbulent transition. The results are expected to contribute to a better understanding of how thermal surface conditions can passively affect transition behaviour, and to assess the potential of such approaches as a basis for future passive boundary-layer control concepts.

Ma [-]	T_∞ [K]	p_∞ [Pa]	Re [-]
7.27	162	2610	10^6 - 10^7

Table 1. T4 shock tunnel operating conditions

ACKNOWLEDGEMENTS

The authors gratefully acknowledge the support by TUM International Graduate School of Science and Engineering (IGSSE) for funding this project, as well as the Leibniz Supercomputing Center for providing the computational capabilities. The authors would also like to thank their project partners at University of Queensland (UQ) for the exchange of configurations and experimental parameters.

REFERENCES

[1] J. B. Vos, N. Duquesne, H. J. Lee, *Proceedings of the 3rd European Symposium on Aerothermodynamics* (1998).
[2] C. Stemmer, M. Birrer, N. Adams, *Journal of Spacecraft and Rockets* **54**, 945–960 (2017).
[3] A. Di Giovanni, C. Stemmer, *Journal of Spacecraft and Rockets* **56**, 1409–1423 (2019).
[4] G. Chiapparino, C. Stemmer, *Int. Journal of Heat and Fluid Flow* **103**, 109193 (2023).
[5] R. Zhao, C. Wen, X. Tian, T. Long, W. Yuan, *Int. Journal of Heat and Mass Transfer* 986–99801 (2018).
[6] R. Ananthapadmanaban, A. Veeraragavan, T. McIntyre, V. Wheatley, D. Mee, *25th AIAA International Space Planes and Hypersonic Systems and Technologies Conference* (2023).

Abstract 101

Collision-Model Effects in DSMC and Implicit PIC Simulations of Rarefied Hypersonic Ionizing Flow

R. J. McDonald[1,a)], J. C. Foster[1], P. Valentini, and A. R. Vazsonyi[2]

[1] *Air Force Institute of Technology, Dayton, OH, USA*
[2] *Air Force Research Laboratory, Albuquerque, NM, USA*
[3]*The Aerospace Corporation, Chantilly, VA, USA*

[a)] Corresponding author: richmond.mcdonald@au.af.edu

Hypersonic reentry at altitudes above 80 km produces a partially ionized shock layer in a regime characterized by a finite Knudsen number (Kn > 0.01), strong thermochemical nonequilibrium, and breakdown of continuum transport assumptions. The Direct Simulation Monte Carlo (DSMC) method remains the standard approach for modeling rarefied hypersonic flows [1, 2]. However, most plasma-capable DSMC implementations rely on the ambipolar diffusion approximation (ADA) to avoid explicit resolution of electron dynamics, an assumption whose validity in strongly ionizing rarefied flows remains under active investigation [3, 4].

This work presents a comparative study between DSMC and an implicit Particle-in-Cell (PIC) formulation applied to a Mach-25 axisymmetric blunt-body reentry configuration at 85.5 km altitude. DSMC simulations are performed using SPARTA with a Variable Hard Sphere (VHS) collision model and Total Collision Energy (TCE) reaction formulation. The PIC simulations employ energy-dependent reaction cross sections derived from Arrhenius rate coefficients, together with a hard-sphere elastic-scattering model. Both solvers implement an identical reduced air-chemistry mechanism and translational-only energy exchange to isolate differences arising from transport and charged-particle treatment.

While both approaches predict similar shock-topology and stagnation-structure patterns, significant discrepancies arise in the shock-layer electron density. The PIC solution predicts electron number densities approximately one order of magnitude higher than the DSMC baseline. Analysis indicates that this difference originates primarily from the elastic scattering model: the hard-sphere formulation overpredicts momentum transfer at high relative velocities, modifying residence times and local reaction rates. The results indicate the sensitivity of rarefied ionizing flows to transport-model selection and highlight the importance of consistent collision physics when coupling plasma kinetics to DSMC-based aerothermodynamics.

ACKNOWLEDGEMENTS

Thank you to the Air Force Research Laboratory for sponsoring this work.

REFERENCES

[1] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows,* (Oxford University Press, Oxford, 1994)
[2] I. D. Boyd, *Journal of Spacecraft and Rockets*, 52, 38-53 (2015).
[3] C. R. Kaplan and E. S. Oran, *Journal of Thermophysics and Heat Transfer*, **36**, 734-744 (2022).
[4] E. D. Farbar and I. D. Boyd, *Physics of Fluids,* **22,** 103103 (2010).

Vibrationally state-resolved rotational relaxation time

Y. Yun[1,a)] and E. V. Kustova[1]

[1] *St Petersburg University, 7-9 Universitetskaya Embankment, St Petersburg, Russia, 199034.*

[a)] Corresponding author: st135205@student.spbu.ru

In high-temperature non-equilibrium flows, the traditional Parker rotational relaxation model [1] based on the rigid rotor assumption cannot accurately describe the effects of internal molecular structure on collision energy transfer. Its applicability to state-to-state modeling is limited when rotational relaxation times depend on vibrational energy levels.

This study develops a new model based on the Variable Hard Sphere (VHS) model and statistical inelastic collision theory [2], accounting for the effects of vibrational state and rovibrational coupling on the cross section of inelastic collisions resulting in the rotational energy transition. An exponential correlation function $S_{jj'll'}(E) = \exp(-\theta'|\Delta E|/E)$ is introduced, where ΔE represents the rotational energy variation upon collision and θ' is a model parameter. Vibrational state-dependent rotational relaxation times were derived through rotational transition cross sections.

Model validation involved comparing Boltzmann-averaged state-to-state relaxation times against other models. Systematic sensitivity analysis revealed a strict linear relationship between the averaged rotational relaxation time and θ', significantly simplifying the parameter fitting procedure. For N_2–N_2, N_2–N, O_2–O_2, and O_2–O systems, optimal θ' values were determined based on recent theoretical data [3–5] with average relative errors below 0.7%. Figure 1 presents the N_2–N rotational relaxation times, comparing the improved model with reference [3], Parker theory, and results without correlation functions, demonstrating excellent agreement with *ab initio* calculations.

The improved model provides a theoretically accurate and computationally efficient tool for calculating state-to-state rotational relaxation times and transport coefficients, with significant implications for aerospace applications including atmospheric reentry simulations.

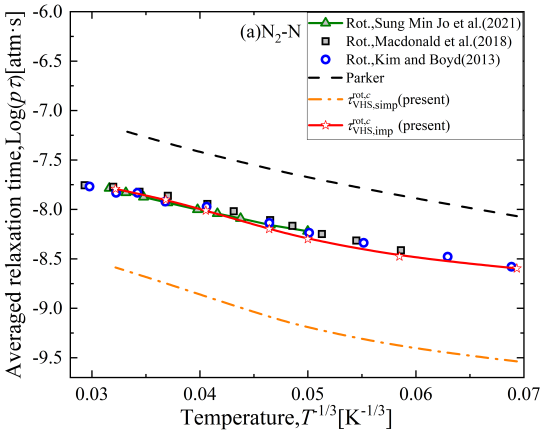


Fig. 1. Comparison of rotational relaxation times in the N_2-N system with simplified model and existing theoretical data.

ACKNOWLEDGEMENTS

The research leading to these results is supported by the Saint Petersburg State University, Project No. 116636233.

REFERENCES

[1] J. Parker, *The Physics of Fluids* **2**, 449–462 (1959).
[2] K. Koura, *Physics of Fluids A: Fluid Dynamics* **4**, 1782–1788 (1992).
[3] S. M. Jo, M. Panesi, J. G. Kim, *Physics of Fluids* **33** (2021).
[4] R. Macdonald, R. Jaffe, D. Schwenke, M. Panesi, *The Journal of chemical physics* **148** (2018).
[5] J. G. Kim, I. D. Boyd, *Chemical Physics* **415**, 237–246 (2013).

State-to-state collision integrals and transport coefficients in oxygen mixtures

Y. Yun[1,a)], Q. Hong,[2] and E. V. Kustova[1]

[1]*St Petersburg University, 7-9 Universitetskaya Embankment, St Petersburg, Russia, 199034.*
[2]*State Key Laboratory of High Temperature Gas Dynamics, Institute of Mechanics, Chinese Academy of Sciences, 100190 Beijing, China.*

[a)]Corresponding author: st135205@student.spbu.ru

Accurate transport coefficients are critical for predicting aerothermal environments during high-speed flight and atmospheric reentry processes. Collision integrals form the foundation for calculating transport coefficients. This study calculates the vibrationally state-resolved transport collision integrals of O_2-O and O_2-O_2 collision systems using the quasi-classical trajectory (QCT) method based on high-accuracy *ab initio* potential energy surfaces (PESs) within the state-to-state kinetic framework. A comprehensive state-resolved dataset of diffusion ($\sigma^2\Omega^{(1,1)*}$) and viscosity ($\sigma^2\Omega^{(2,2)*}$) collision integrals is provided over the temperature range of 1000-20000 K.

The results demonstrate that vibrational excitation strongly influences collision integrals and rotational energy transfer, with effects becoming more pronounced at high temperatures. Collision integrals differ by up to 50% between ground and highly excited vibrational states, and exhibit significant differences from the results of Subramaniam et al. [1] at high temperatures. The calculated collision integrals are validated against experimental data at low and moderate temperatures, showing good agreement with measured shear viscosity and thermal conductivity. Figure 1 presents comparison with traditional models [2–6] reveals temperature-dependent discrepancies.

The present quantitative analysis of vibrational-state effects on collision integrals delineates the applicability limits of different phenomenological models and provides high-precision data for computational fluid dynamics simulations of high-speed flows.

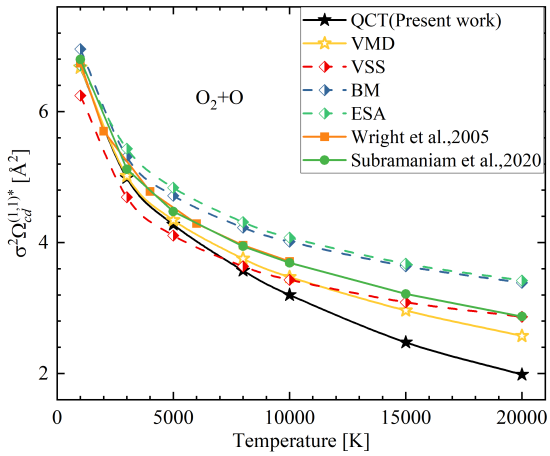


Fig. 1. Boltzmann-averaged results from traditional models and QCT method.

ACKNOWLEDGEMENTS

The work of Y. Yun and E. Kustova was supported by Saint Petersburg State University, Project No. 116636233.

REFERENCES

[1] S. Subramaniam, R. L. Jaffe, K. A. Stephani, *Physical Review Fluids* **5**, 113402 (2020).
[2] E. V. Kustova, G. M. Kremer, *Chemical Physics Letters* **636**, 84–89 (2015).
[3] A. B. Weaver, A. A. Alexeenko, *Journal of Physical and Chemical Reference Data* **44** (2015).
[4] S. J. Cubley, E. Mason, *The Physics of Fluids* **18**, 1109–1111 (1975).
[5] A. Laricchiuta, G. Colonna, D. Bruno, R. Celiberto, C. Gorse, F. Pirani, M. Capitelli, *Chemical Physics Letters* **445**, 133–139 (2007).
[6] M. J. Wright, D. Bose, G. E. Palmer, E. Levin, *AIAA journal* **43**, 2558–2564 (2005).

DSMC study of shock waves based on the state-resolved rotational relaxation model

L. Tan[1,a)], **Y. Yun**[1] and E. V. Kustova[1]

[1] *St Petersburg University, 7-9 Universitetskaya Embankment, St Petersburg, Russia, 199034.*

[a)] Corresponding author: st088860@student.spbu.ru

Shock wave structures in hypersonic flows are strongly influenced by rotational energy relaxation processes [1]. The widely-used Parker model, however, underpredicts density in the near-shock region compared to experiments, due to its inability to capture the vibrational state dependence of rotational energy transfer. This limits the model's accuracy in predicting shock wave profiles and internal energy distributions.

This work evaluates a vibrationally state-resolved rotational relaxation model [2] for N_2 and O_2 normal shock wave simulations using the Direct Simulation Monte Carlo (DSMC) method. The model, based on the Variable Hard Sphere (VHS) model and Statistical Inelastic Cross Section (SICS) theory, employs an exponential correlation function $S_{jj'll'}(E) = \exp(-\theta'|\Delta E|/E)$ to describe transition probabilities between rotational energy states in molecular collisions. In this work, the model is efficiently integrated into the DSMC framework through a temperature-dependent rotational collision number $Z_{\mathrm{rot}}(T)$ constructed from pre-calculated state-resolved relaxation times.

Normal shock wave simulations were performed across multiple Mach numbers in nitrogen and oxygen, where high temperatures lead to molecular dissociation. Figure 1 presents translational temperature, rotational temperature, and density profiles for shock waves in nitrogen molecular-atomic (N_2–N) at $M = 10$, comparing the state-resolved model (VHS-SICS model) with the classical Parker model [3] and experimental data from Alsmeyer [4]. The results demonstrate that the vibrationally state-resolved model significantly improves prediction accuracy over the Parker model, showing excellent agreement with experimental measurements and better capturing the vibrational-rotational coupling effects in the shock structure. This evaluation validates the applicability of advanced state-resolved rotational relaxation models for high-fidelity hypersonic flow simulations.

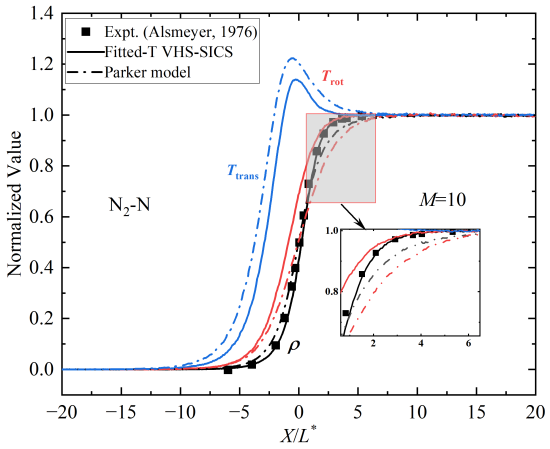


Fig. 1. Comparison of rotational relaxation models against experimental data for N_2–N shock waves at $M = 10$. Blue lines: translational temperature (T_{trans}); red lines: rotational temperature (T_{rot}); black symbols and lines: density (ρ). The inset shows a magnified view of the near-shock region.

ACKNOWLEDGEMENTS

The research leading to these results is supported by the Saint Petersburg State University, Project No. 116636233.

REFERENCES

[1] P. Valentini, C. Zhang, T. E. Schwartzentruber, *Physics of Fluids* **24** (2012).
[2] Y. Yun, E. Kustova, *The Journal of Chemical Physics* **163** (2025).
[3] J. Parker, *The Physics of Fluids* **2**, 449–462 (1959).
[4] H. Alsmeyer, *Journal of Fluid Mechanics* **74**, 497–513 (1976).

Gas-Dynamic Characterization of Airlock Venting Operations and Outgassing from Manned Lunar Rovers

S. Boccelli[1,a)], W.M. Farrell[2,3], P. Saxena[4] and O.J. Tucker[4,5]

[1]*NPP Postdoctoral Fellow, NASA GSFC, 8800 Greenbelt Rd, Greenbelt, 20771 Maryland, USA*
[2]*Space Science Institute, 4765 Walnut Street, Suite B, Boulder, CO 80301, USA*
[3]*DeepSpace Technologies Inc., 8865 Stanford Boulevard, Suite 183, Columbia, MD 21045, USA*
[4]*NASA Goddard Space Flight Center, 8800 Greenbelt Rd, Greenbelt, 20771 Maryland, USA*
[5]*Department of Atmospheric and Planetary Sciences, Hampton University, Hampton, VA 23668, USA*

[a)]Corresponding author: stefano.boccelli@nasa.gov

A multitude of international efforts towards lunar exploration are currently underway. In the US, the Commercial Lunar Payload Services (CLPS) program and the Artemis missions are bringing robotic payloads and manned spacecraft to the moon. These exploration activities carry a great science potential, but an equally large risk of anthropogenic contamination of the pristine lunar environment, which might prevent science objectives to be met [1]. Lunar-rover modules (see Fig. 1) are presently being designed in support to the Artemis missions. These modules, maintained at breathable pressure levels, will provide a habitat to the astronauts for multiple Earth days and contain a variety of life-support payloads, as well as externally-exposed radiators, solar panels and an airlock section to allow for Extravehicular Activities (EVAs) [2].

In this work, after analyzing possible depressurization scenarios, we perform Direct Simulation Monte Carlo (DSMC) studies of the air discharge from the airlock to the lunar exosphere and characterize the spatial extent and magnitude of the resulting particle fluxes on the regolith. During the depressurization process, the flow evolves from the continuum regime, inside the airlock and near the vent, to free-molecular conditions and rarefaction-capable methods are necessary. Besides venting, outgassing is also expected to be a major contamination factor, as previously demonstrated by the LACE mass spectrometer deployed during the Apollo missions. In this case, outgassing was observed to be so prevalent as to swamp any measurements during the lunar day [3]. We analyze here outgassing from the Multi-Layer Insulation (MLI) blanketing and from solar panels, adopting available outgassing rates from the literature. Owing to the lower density involved, outgassing is studied here using a view-factor method.

By comparing our results with the natural abundances of exospheric species [4], we provide an indication of how far scientific measurements should be carried from the module. We find that, depending on the actual outgassing rates, contamination might be prevalent up to distances of kilometers from the module.

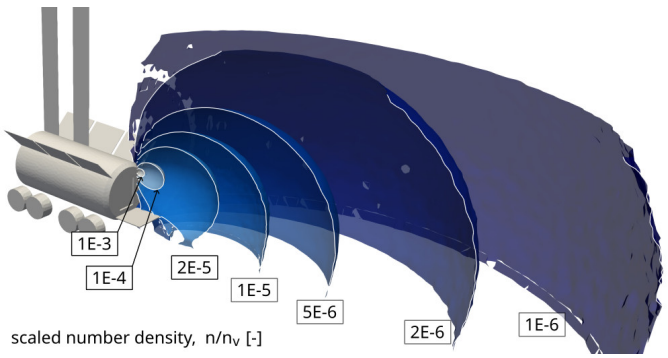


Figure 1: DSMC simulation of an airlock depressurization process. Local number density contours, scaled with the density at the vent.

REFERENCES

[1] R. M. Killen, L. Yeo, Y. Zheng, J. Mclain, J. Marshall, L. Morrissey, C. Ahrens, P. Phipps, H. Graham, T. J. Stubbs, *Bulletin of the American Astronomical Society* **56** (2024).
[2] S. Illiano, R. Mugnuolo, M. Musmeci, L. Ansalone, F. Vagnone, N. Genco, F. Fenoglio, T. Nickens, E. Alexander, *International Astronautical Congress 2024, Milan* (IAF, 2024), IAC–24,B3,1,2,x86708.
[3] S. A. Stern, *Reviews of Geophysics* **37**, 453–491 (1999).
[4] W. M. Farrell, J. S. Halekas, M. Horányi, R. M. Killen, C. Grava, J. R. Szalay, M. Benna, P. E. Clark, M. R. Collier, A. Colaprete *et al.*, *Reviews in Mineralogy and Geochemistry* **89**, 563–609 (2023).

[POSTER PRESENTATION] Comparing Multi-Species BGK Models with DSMC for Rarefied Subsonic, Transonic and Supersonic Flows

S. Boccelli[1,a)], A. Macaluso[2] and G. Martalò[3]

[1]*NPP Postdoctoral Fellow, NASA Goddard Space Flight Center, 8800 Greenbelt Rd, Greenbelt, 20771 Maryland, USA*
[2]*Dipartimento di Scienze Matematiche, Fisiche e Informatiche, Università di Parma, Parco Area delle Scienze 53/A, 43124 Parma, Italy*
[3]*Dipartimento di Matematica "Felice Casorati", Università di Pavia, Via Ferrata 5, 27100 Pavia, Italy*

[a)]Corresponding author: stefano.boccelli@nasa.gov

While approximated, Bhatnagar-Gross-Krook (BGK) collision models [1] allow for a simpler implementation as compared to the full Boltzmann collision operator. Moreover, various rarefied-fluid-dynamic models cannot deal with the Boltzmann operator. This is the case for the maximum-entropy moment method for instance, or for other moment closures where the distribution function is not readily available. For such methods, employing BGK-like operators is a practical necessity.

The accuracy of the BGK collision operator for a single-species gas has been extensively analyzed in the past and ample literature is available. However, few studies exist for gas mixtures. In this work, we consider a general formulation of the multi-species BGK operator [2], which extends the previous formulations [3] by including multiple intermediate relaxation states. The model has so far been only analyzed in spacially-homogeneous or one-dimensional cases.

We first perform numerical simulations in 0D, analyzing the relaxation of a helium-argon binary mixture. We then consider multi-dimensional test cases of rarefied gas flows past a solid object at different Mach numbers and compare the multi-species BGK results to full Direct Simulation Monte Carlo (DSMC) simulations. Our results permit to identify the strengths and limitations of this model and suggest further directions of development.

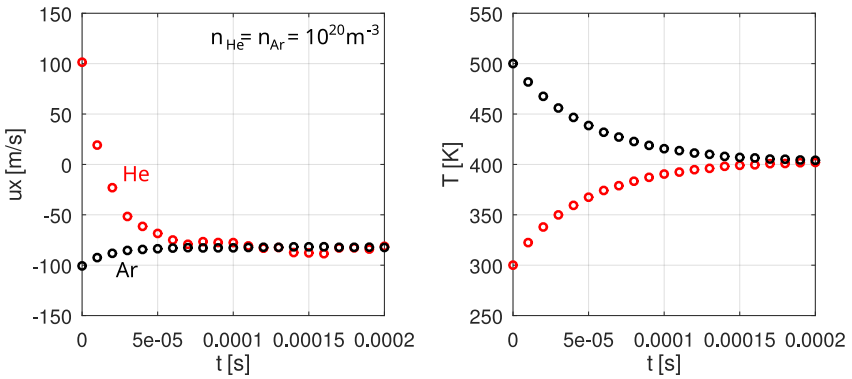


Figure 1: relaxation of a helium-argon mixture in 0D predicted with DSMC. In this work we will compare these DSMC calculations with results from the multi-component BGK model in 0D and for 2D test cases.

ACKNOWLEDGEMENTS

SB's work was supported by an appointment to the NPP Postdoctoral Program, held at NASA Goddard Space Flight Center and administered by Oak Ridge Associated Universities under contract with NASA.

REFERENCES

[1] P. L. Bhatnagar, E. P. Gross, M. Krook, *Physical review* **94**, 511 (1954).
[2] A. V. Bobylev, M. Bisi, M. Groppi, G. Spiga, I. F. Potapenko, *Kinetic & Related Models* **11** (2018).
[3] P. Andries, K. Aoki, B. Perthame, *Journal of Statistical Physics* **106**, 993–1018 (2002).

Abstract 107

Experimental Heat Transfer Distributions in Swept Shock-Boundary Layer Interactions (SwSBLIs) across Rarefied Regimes

N. F. Anyamele[1,a)], N. Donaldson[2,1], A. Berry[1], P. T. Ireland[1], and L. J. Doherty[1]

[1] *Oxford Thermofluids Institute, University of Oxford, Osney Mead, Oxford, OX2 0ES.*
[2] *Fluid Gravity Engineering Ltd., Emsworth, PO10 7DX.*

[a)] Corresponding author: nnaemeka.anyamele@eng.ox.ac.uk

Spaceplanes and aircraft designed for point-to-point hypersonic travel can be designed for a variety of trajectory options which may involve travel at or across regions of high altitudes [1]. These vehicles are therefore expected to experience conditions that span degrees of rarefaction.

The present work investigates the macroscopic impacts of wings and aerodynamic controls surfaces on aircraft performance over varying extents of rarefaction. The presence of aerodynamic surfaces give rise to complex flow phenomena, specifically shock-shock interactions (SSIs) and shock-boundary layer interactions (SBLIs) [2]. Several canonical interaction cases have received much attention in recent decades, in both continuum and rarefied regimes, such as the double cone [3], the compression corner [4], and Edney type shock-shock interactions [5].

One broad category of SSI/SBLI that has received very little experimental investigation at rarefied conditions are swept shock-boundary layer interactions (SwSBLIs), which occur when fluid flows super-/hypersonically in the corner of two intersecting surfaces in a direction generally parallel to the axis of the intersection. Due to their complexity, accurate computational simulation of SBLIs have historically required extensive effort, relying heavily on good experimental data for validation [3]. It is understood that the complex, and often detrimental, flow structures that develop in SwSBLIs (and most SBLIs) at continuum conditions should eventually break down at sufficiently rarefied conditions. However, the exact degree of rarefaction that this break down occurs is not well established; this may influence both the extent to which a skipping trajectory may periodically re-enter the atmosphere and the future design of these aircraft to make better and safer use of the atmosphere in such trajectories.

This paper reports on experiments conducted in the Low Density Tunnel (LDT) of the Oxford Thermofluids Institute. Liquid Crystal Thermography (LXT) is used to ascertain how the heat transfer distribution over various corner geometries vary due to the presence of varying intensities of SwSBLIs as the degree of rarefaction varies. LXT has recently been used in LDT to investigate heat transfer on geometries in the context of satellite demise [6]. The LDT was designed to carry out investigations in the slip/transition regimes, and thus offers the exclusive potential to explore the likely break down regimes in a way that cannot yet be achieved accurately or inexpensively by CFD and DSMC. While both tools have been shown to eventually achieve decent results in these regimes for other investigations, it remains the primary task to gather experimental data.

ACKNOWLEDGEMENTS

This research was funded and supported by Dstl.

REFERENCES

[1] K. Zhang, W. Chen, *Proc. of the 17th AIAA International Space Planes and Hypersonic Systems and Technologies Conference* (AIAA, San Francisco, CA, USA, 2011).
[2] H. Babinsky, J. K. Harvey, *Shock Wave-Boundary-Layer Interactions* (Cambridge University Press, Cambridge, 2011).
[3] J. K. Harvey, M. S. Holden, T. P. Wadhams, *Proc. of the 39th AIAA Aerospace Sciences Meeting* (AIAA, Reno, NV, USA, 2001).
[4] Ch-H. Chun, *Proc. of the 17th Int'l Symposium on Rarefied Gas Dynamics* (Hoboken, NJ, USA, 1990) pp. 562–569.
[5] V. Cardona, R. Joussot, V. Lago, *Experiments in Fluids*, **62**(135), pp. 1–14 (2021).
[6] N. Donaldson, *Hypersonic Modelling and Testing of Space Debris During Planetary Entry* (PhD Thesis, University of Oxford, 2019)

Abstract 108

Rarefaction effects on high-speed boundary-layer stability and receptivity

Jihui Ou[1,a)], Jie Chen[1]

[1]*Department of Mechanics, Tianjin University, Tianjin, 300072, China*
[a)] Corresponding author: oujihui@tju.edu.cn

The boundary-layer transition problem has always raised much attention and not been well resolved. For high-speed flows at high altitudes, such as at 40-60 km, the boundary-layer transition might still occur while local rarefaction effects exist in the boundary layer. The rarefaction effects cause the failure of the continuum hypothesis and the conventional Navier-Stokes (NS) equations, and can influence the boundary-layer stability and receptivity, which has rarely been studied. In this report, the high-speed boundary-layer stability and receptivity to free-stream acoustic waves over a flat plate (at Mach numbers 4.5~10) in near-continuum regime are studied, and the rarefaction effects on the boundary-layer stability and receptivity are clarified. The main results are as follows: 1) an extended linear stability theory is developed by considering surface slip effects and nonlinear constitutive relations in the macroscopic framework, and unified gas kinetic simulation (UGKS) is also performed to track the disturbance evolution; 2) for the stability, the rarefaction effects delay the synchronization between slow and fast modes, stabilize the second-mode instability while destabilize the first-mode instability; 3) for the receptivity, the slip effects can cause the receptivity coefficient increasing by 25%, which depends on the receptivity route; 4) the kinetic simulation recovers to the conventional linear stability results in the continuum regime, and confirms the extended stability method in near-continuum regime.

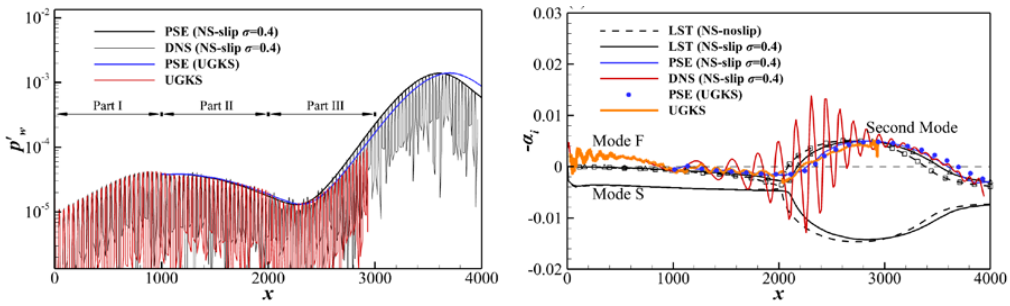


Fig. 1 Distributions of surface pressure perturbations and disturbance growth rate by different methods (*Ma*=4.5)

ACKNOWLEDGEMENTS

This work was supported by the National Natural Science Foundation of China under grant numbers 12202307, 12472336 and 92471106.

REFERENCES

[1] Chenyue Wang, Jihui Ou, Jie Chen, *Physics of Fluids*, **36**, pp. 094125 (2024).
[2] Jihui Ou, Chenyue Wang, Jie Chen, *Acta Mechanica Sinica*, **40**, pp. 123184 (2024).

A modeling framework for gas-surface interaction processes in hypersonics and plasma discharges

A. Munafò[1,a)], C. Chicchiero[1], A. Singh[1], S. Kumar[1], K. Stephani[1] and M. Panesi[1]

[1]*Department of Mechanical and Aerospace Engineering, University of California, Irvine, CA 92697, USA*

[a)]Corresponding author: amunafo@uci.edu

The calculation of multi-component reactive flows such as those found in hypersonics and plasma discharges requires a theoretical framework encompassing non-equilibrium thermodynamics, transport phenomena, collisional-radiative kinetics as well as gas-surface interaction (GSI) processes. In most of applications the fluid may be considered as a *continuum* and modeled as a collection of dilute gases. Under these circumstances, the hydro-dynamic equations and the associated constitutive relations may be rigorously obtained based on Kinetic Theory [1, 2].

In the last two decades significant efforts have been devoted towards the development of accurate GSI models for thermal protection system (TPS) materials [3]. The inclusion of GSI requires taking into account phenomena such as pyrolysis, ablation and sublimation, which adds further complexity to the modeling [4, 5]. In analogy with the multi-temperature formulations for gas-phase kinetics mainly developed during the 1980's, the first models for GSIs were also correlation-based and, as such, have a limited domain of applicability [3]. At the present time, these legacy models are being replaced by more accurate formulations which describe the interaction between a high-temperature multi-component gas and a surface in terms of elementary processes (*e.g.*, adsorption, desorption) [6–8].

The purpose of this work is the development of a theoretical and computational framework for GSIs under conditions relevant for hypersonics and plasma discharges. To achieve self-consistency, the surface mass balance relations accounting for processes such as adsorption and dissociative chemisorption are incorporated into Stefan-Maxwell's equations stemming from Kinetic Theory.

Instead of adopting a monolithic approach, the multi-physics framework for studying GSIs is built based on the coupling of stand-alone solvers - developed either by the authors or by external collaborators - responsible for: (i) the flowfield, (ii) the material (*e.g.*, TPS sample) and (iii) the electromagnetic field.

The fluid governing equations are numerically solved using HEGEL, a finite volume solver for multi-component gases and plasmas [9]. HEGEL currently relies on the PLATO library [10] for computing all gas-related quantities (*e.g.*, transport properties). The evolution of the material's temperature, composition and shape resulting from the interaction with the surrounding reactive fluid is simulated by utilizing PATO [11], a finite volume solver for porous materials. Electromagnetic phenomena are handled by FLUX [12, 13], a finite element software for time- and frequency-domain electromagnetic problems. The exchange of information (*e.g.*, coupling) among the three solvers is accomplished via PRECICE, an open source library for partitioned multi-physics simulations [14].

ACKNOWLEDGEMENTS

This work is funded by the Vannevar Bush Faculty Fellowship OUSD(RE) (Grant No: N00014-21-1-295).

REFERENCES

[1] V. Giovangigli, *Multicomponent Flow Modeling* (Birkhäuser, Berlin, 1999).
[2] E. Nagnibeda, E. Kustova, *Non-Equilibrium Reacting Gas Flows* (Springer, Berlin, 2009).
[3] G. Duffa, *Ablative Thermal Protection Systems Modeling*, AIAA Education Series (American Institute of Aeronautics and Astronautics, 2013).
[4] J. Marschall, M. MacLean, *AIAA Paper 2011-3783* (June 2011), 10.2514/6.2011-3783.
[5] M. MacLean, J. Marschall, D. Driver, *AIAA Paper 2011-3784* (June 2011), 10.2514/6.2011-3784.
[6] S. V. Zhluktov, T. Abe, *J. Thermophys. Heat Transfer* **13**, 50–59 (1999).
[7] K. Swaminathan-Gopalan, K. A. Stephani, *AIP Adv.* **9**, 035246 (2019).
[8] K. S. Prata, T. E. Schwartzentruber, T. J. Minton, *AIAA J.* **60**, 627–649 (2022).
[9] A. Munafò, S. M. Jo, S. Kumar, M. Panesi, *AIAA Paper 2024–0449* (January 2024), 10.2514/6.2024-0449.
[10] A. Munafò, M. Panesi, *J. Thermophys. Heat Transfer* **39**, 850–870 (2025).
[11] J. Lachaud, N. N. Mansour, *J. Thermophys. Heat Transfer* **28**, 191–202 (2014).
[12] S. Kumar, A. Munafò, V. Le Maout, N. Mansour, M. Panesi, *AIAA Paper 2022–1619* (January 2022), 10.2514/6.2022-1619.
[13] S. Kumar, A. Munafò, S. M. Jo, M. Panesi, *J. Phys. D: Appl. Phys.* **58**, 025204 (2024).
[14] G. Chourdakis, K. Davis, B. Rodenberg, M. Schulte, F. Simonis, B. Uekermann, G. Abrams, H. Bungartz, L. Cheung Yau, I. Desai, K. Eder, R. Hertrich, F. Lindner, A. Rusch, D. Sashko, D. Schneider, A. Totounferoush, D. Volland, P. Vollmer, O. Koseomur, *Open Research Europe* **2** (2022), 10.12688/openreseurope.14445.2.

Effect of Adsorbed Molecules on the Scattering Characteristics of Gas Molecules at Solid Surfaces

Kazuki Takemura[1], Takashi Tokumasu[2], and Hideki Takeuchi[1,a)]

[1] *National Institute of Technology, Kochi College, Nankoku, 783-8508, JAPAN.*
[2] *Institute of Fluid Science, Tohoku University, Sendai, 980-8577 JAPAN.*

[a)] Corresponding author: takeuchi@me.kochi-ct.ac.jp

In high Knudsen number flows, gas-surface scattering plays an important role in determining macroscopic thermal and flow properties. Accordingly, an accurate description of gas-surface interactions is essential for their analysis. In many practical simulations, diffuse reflection is commonly employed as the gas-surface boundary condition; however, this assumption is not necessarily valid for extremely clean surfaces, high surface temperatures, or high flow velocities. In recent years, scattering kernel for monoatomic gases have been proposed on scattering characteristics at solid surfaces with physisorbed molecules [1], and gas-surface scattering of diatomic gases has been investigated using the molecular dynamics (MD) method, focusing on the effects of adsorbed molecules and surface roughness on accommodation coefficients [2]. In the present study, nitrogen gas, a diatomic molecule with internal degrees of freedom, is analyzed by a hybrid approach that combines the MD method with the direct simulation Monte Carlo (DSMC) method [3]. The effects of macroscopic flow conditions and atomic-scale surface characteristics of solid surfaces with adsorbed molecules different from the gas species on gas-surface scattering behavior are evaluated and discussed.

As in the previous study [3], a Couette flow of nitrogen (N_2) gas between two parallel plates separated by a distance L is considered. The upper and lower plates move at velocities of $-U/2$ and $U/2$, respectively, and are maintained at a temperature of T_W = 300 K. The motion of gas molecules between the plates is simulated using the DSMC method. When a gas molecule collides with a solid surface in the DSMC simulation, its post-collision velocity and rotational energy are determined though a MD simulation. The intermolecular potentials for both gas-gas and gas-solid interactions are identical to those employed in our previous studies [3, 4]. The solid surface is assumed to be atomically flat (smooth). Three types of solid surfaces are considered: a clean platinum (Pt) surface, and Pt surfaces with adsorbed xenon (Xe) atoms or water (H_2O) molecules.

Figure 1 shows the distribution of the flow velocity, $q_x/(U/2)$ for K_n = 0.2 and S = 1.0. Here, $K_n = \lambda/L$ is the Knudsen number and $S = (U/2)/C_m$ is the speed ratio of the wall, where λ denotes the mean free path of gas molecules at equilibrium, and C_m is the most probable speed of gas molecules corresponding to the wall temperature T_W. The horizontal axis represents the nondimensional distance from the lower wall, where Y/L = 0 corresponds to the lower surface. Owing to symmetry about the channel centerline, only the flow velocity distribution from the lower wall to the centerline is presented. The velocity slip at the lower plate decreases in the order of the Xe adsorbed surface, the H_2O adsorbed surface, and the clean surface.

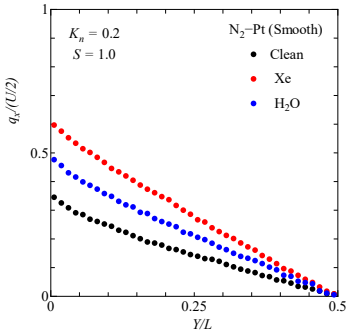


Fig. 1. Flow velocity distributions.

ACKNOWLEDGEMENTS

This work was supported by JSPS KAKENHI Grant Number JP25K07593.

REFERENCES

[1] Y. Chen, L. Gibelli, and M. Borg, Impact of Surface Physisorption on Gas Scattering Dynamics, *J. Fluid Mech.*, **968**, A4 (2023).
[2] Q. Miao, L. Li, X. Yu, J. Wu, and M. Fang, Molecular Dynamics Insights into Reflected Gas Behavior in Rarefied Flow: Effect of Gas-Surface Interaction Strength and Surface Conditions, *Surfaces and Interfaces*, **71**, 106884 (2025).
[3] K. Yamamoto, H. Takeuchi, and T. Hyakutake, Characteristics of Reflected Gas Molecules at a Solid Surface, *Phys. Fluids*, **18**, 046103 (2006).
[4] N. Uene, H. Takeuchi, Y. Hayamizu, and T. Tokumasu, Study of Reflection Models of Gas Molecules on Water Adsorbed Surfaces in High-Speed Flows, *Journal of Fluid Science and Technology*, **15** (1), JFST0005 (2020).

Abstract 111

R&D Activity on the Inflatable Aeroshell Atmospheric-entry Technology and Future Vision of Mars Exploration

Kazuhiko Yamada[1,a)]

[1] Japan Aerospace Exploration Agency,
3-1-1 Yoshinodai, Sagamihara chuo-ku, Kanagawa, 252-5210, Japan

[a)] Corresponding author: yamada.kazuhiko@jaxa.jp

An inflatable aeroshell technology is increasingly attracting attention as the next generation of atmospheric-entry technology. Research and development on the inflatable aeroshell in Japan started in 2000 from preliminary study at Kojiro Suzuki laboratory, The university of Tokyo. This activity has been led by Prof. Kojiro Suzuki from that time until the present. The unique feature of this activity is that it has progressed with various flight tests as its milestone.

The first big milestone of this R&D is free flight tests using large scientific balloons. These flight tests were carried out in 2003 and 2004. In these tests, a capsule-type vehicle with a large and low-mass flexible aeroshell was demonstrated to fly stable in transonic speed regime[1]. Following the balloon drop test, the reentry demonstration using a sounding rocket (S-MAAC) was carried out in 2012 (Figure 1). In this demonstration, the deployment of 1.2m inflatable aeroshell in vacuumed and zero-gravity environment and reentry flight from altitude of 150km was demonstrated successfully[2]. In 2017, the 3U nano satellite EGG was developed to demonstrate the deployment of inflatable aeroshell in LEO and rapid orbital decay with a large and low-mass aeroshell (Figure 2) [3]. The inflatable aeroshell technology matured by utilizing the various flight tests.

Inflatable aeroshell technology has a strong advantage for Mars landing exploration where the atmosphere is thin, because this technology can utilize aerodynamic force efficiency. Therefore, the R&D team led by Prof. Kojiro Suzuki proposed an innovative Mars exploration concept “SPUR” that is network-type exploration by scattered many small probes. This concept becomes a base of STEP1 mission in stepwise Mars exploration program discussed in JAXA now. In this paper, the history of the R&D on the inflatable aeroshell and future vision of Mars exploration utilizing the inflatable aeroshell technology are introduced.



Fig. 1 Group photo of S-MAAC team in 2012. (Prof. Kojiro Suzuki is shown in at center right)



Fig. 2 Successful deployment of nano-satellite EGG and Prof. Kojiro Suzuki celebrating it, in 2017

REFERENCES

[1] Yamada, K., Akita D., Sato, E., Suzuki, K., Narumi, T., and Abe, T.:Flare-Type Membrane Aeroshell Flight Test at Free Drop from a Balloon, J. Spacecraft and Rocket, Vol. 46, No. 3, 2009, pp. 606-614

[2] Yamada, K., Nagata, Y., Abe, T., Suzuki, K., Imamura, O., and Akita,D.: Suborbital Reentry Demonstration of Inflatable Flare-Type Thin-Membrane Aeroshell Using a Sounding Rocket, AIAA Journal of Spacecraft and Rockets, January, Vol. 52, No. 1(2015) : pp. 275-284

[3] Kazuhiko Yamada, Takahiro Moriyoshi, Kazushige Matsumaru, Hiroki Kanemaru, Takahiro Ayara, Kojiro Suzuki, Osamu Imamura, Daisuke Akita, Yasunori Nagata, Yasumasa Watanabe, “Overall Achievements of the Flight Demonstration of EGG: Re-entry Nano-Satellite with Gossamer Aeroshell and GPS/Iridium”, Transactions of the Japan Society for Aeronautical and Space Sciences, Vol. 67, No. 4, Pages 224-233, July, 2024

Modeling of Sawtooth-Shaped Walls for Rarefied Gas Flow Control

J. Lee[1,a)], D. Satpathy[1], K. Komurasaki[1], N. Barth[1], M. Matsukura[1] and H. Koizumi[1]

[1]*The University of Tokyo, Japan*

[a)]Corresponding author: l.jiwon@al.t.u-tokyo.ac.jp

To improve the performance of space propulsion systems, particularly Hall thrusters, various methods to control neutral particle dynamics via injection methods, thermal management, and wall shaping have been proposed. In particular, sawtooth-shaped walls have proven effective in maximizing particle density and lowering average velocity by promoting intentional backflow. This study introduces a novel Sawtooth-CLL model designed to reproduce the reflection distribution of a sawtooth wall. We performed geometric optimization to increase backflow by isolating the effect of the sawtooth inclination angle from other parameters. Furthermore, by introducing an 'effective angle' parameter, the model accurately reproduces the asymmetric reflection distribution inherent to sawtooth geometries. Ultimately, the proposed model predicts an optimal inclination angle of approximately 30 °, providing a significant advantage by simplifying the complex modeling process and minimizing the computational cost of simulations involving small-scale geometries.

Abstract 113

Study of coating uniformity and axis switching of metal vapour jet through rectangular nozzles in thin film deposition systems

A. Mazumder[1,2a)], N. Alangi[1], S. Sethi[3], U. Bhandarkar[4], K. Dasgupta[5], and A. Agrawal[4]

[1] *Beam Technology Development Group, Bhabha Atomic Research Centre, Mumbai-400085, India.*
[2] *Homi Bhabha National Institute, Anushaktinagar, Mumbai-400094, India.*
[3] *Heavy Water Division, Bhabha Atomic Research Centre, Mumbai-400085, India.*
[4]*Department of Mechanical Engineering, Indian Institute of Technology Bombay, Mumbai, India.*
[5] *Materials Group, Bhabha Atomic Research Centre, Mumbai-400085, India.*
[a)] Corresponding author: anikm@barc.gov.in

Thin films of metallic Ytterbium (Yb) and Ytterbium oxide are widely used for applications like LEDs, solar cell, opto-electronics, nanotechnology etc. Experimental investigation and DSMC simulations were carried out to study the sublimation and coating uniformity of metallic Yb through nozzles of rectangular openings inside a PVD system. The study was carried out with nozzles having converging, straight and diverging cross-sections and identical openings in the Knudsen number (Kn) range of $0.05 \leq Kn \leq 5$. The evaporation of Yb was carried out using a Titanium crucible as a reservoir of metal vapour. The DSMC solver was validated using these in-house experimental data for the mass flow rate and spatial distribution of vapour flux. Specular reflection of metal vapour from hot Titanium surface was found to be a close representation of experimental conditions. Preferential scattering of Yb atoms towards specular direction from hot metallic surface was identified as the probable reason for this observation. DSMC results were found to be in good agreement with experimental data with a maximum deviation of 6% for the mass flow rate and 8% for the mass flux distribution. The coating uniformity contour shows maximum radial spread for the converging nozzle and minimum spread for the diverging nozzle. This phenomenon can be attributed to the higher local pressure inside the nozzle due to a different reflection pattern. The major and minor axes of the metal vapour jet were found to be rotated by 90° in converging and straight nozzle similar to axis switching phenomena in continuum jet. However, the phenomenon can be attributed to anisotropic expansion due to steep pressure gradient in the short side and not to the vorticity. For identical Knudsen number, axis switching was observed at a smaller distance from the nozzle for converging nozzle than the straight nozzle. The distance increases with increasing Knudsen number. No axis switching was observed for diverging nozzle in the range of distances and Knudsen number considered for this study. The phenomenon of axis switching in vacuum evaporation has not been reported earlier.

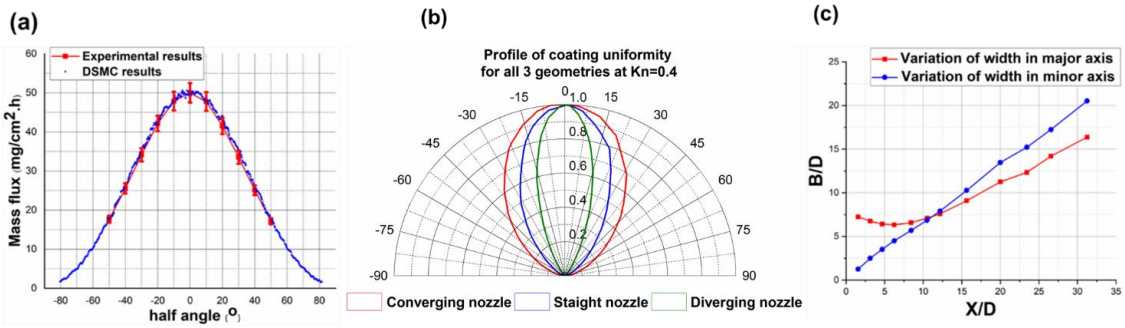


Figure 1. (a) Experimental validation of DSMC solver (b)Comparison of coating uniformity for different nozzle geometry (c) Variation of jet width in major and minor axis for converging nozzle showing axis switching

ACKNOWLEDGEMENTS

Authors acknowledge the support and guidance provided by Shri S. P. Dey and Shri Martin Mascarenhas. Authors are thankful for the funding provided by Board of Research in Nuclear Sciences (BRNS) for this study. Amit Agrawal is grateful to ANRF for J C Bose National Fellowship.

REFERENCES

[1] A. Agrawal, L. Djenidi, and R. A. Antonia, *Journal of Fluid Mechanics*, **530**, pp. 135-144 (2005).
[2] V. Hemadri, V. V. Varade, A. Agrawal, and U. V. Bhandarkar, *Physics of Fluids*, **28**, (2016).
[3] O. Sazhin, and A. Sazhin, *International Journal of Heat and Mass Transfer*, **203**, 123842 (2023).
[4] A. Venkattraman, and A. A. Alexeenko, *Vacuum*, **86**, pp. 1748-1758 (2012).

Surrogate-Based Aerodynamic Shape Optimization of HTV-2-Type Vehicle from Continuous to Rarefied Flow Regimes

Wenpei Long[1,a)], Xiaozhe Xi[1], Yue Zhang[1], Junzhe Cao[1] and Kun Xu[1,2,3]

[1]*Department of Mathematics, The Hong Kong University of Science and Technology, Hong Kong, China*
[2]*Department of Mechanical and Aerospace Engineering, The Hong Kong University of Science and Technology, Hong Kong, China*
[3]*HKUST Shenzhen Research Institute, Shenzhen, 518057, China*

[a)]Corresponding author: wlongab@connect.ust.hk

In the conceptual design of hypersonic vehicles, aerodynamic optimization is essential for evaluating performance to satisfy mission requirements across varying altitudes. To enable effective optimization under these complex conditions, an efficient multiscale simulation method is required to supply accurate aerodynamic data in all flow regimes for model construction and optimization.

In this work, a surrogate-based optimization framework is developed for efficient aerodynamic shaping of a HTV-2-type hypersonic vehicle. The framework adopts the unified gas-kinetic scheme (UGKS)[1] to resolve rarefied and nonequilibrium flow physics. The present scheme employs implicit macroscopic governing equations and couples them with implicit microscopic governing equations within the nonequilibrium region, achieving high convergence efficiency in all flow regimes[2, 3]. To address the challenges of high computational cost, a new UGKS programming paradigm is proposed to reduce memory usage and improve parallel efficiency[4]. These improvements allow each simulation to be completed within 4 hours on a 96-core CPU cluster.

Using the UGKS dataset, a Kriging surrogate model is constructed via MaxiMin Latin Hypercube Sampling (LHS) in the design space. This model links the 5 bottom shape parameters of the vehicle to the single objective of maximizing lift-to-drag ratio, and enforces center of pressure location as a stability constraint. To investigate the rarefied gas effects on optimal vehicle shaping, the framework is applied to the vehicle across altitudes corresponding to different flow regimes.

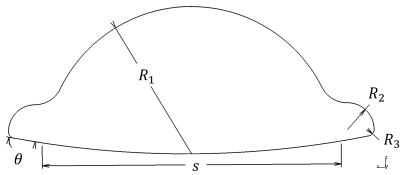


Fig. 1. Schematic of bottom shape parameters.

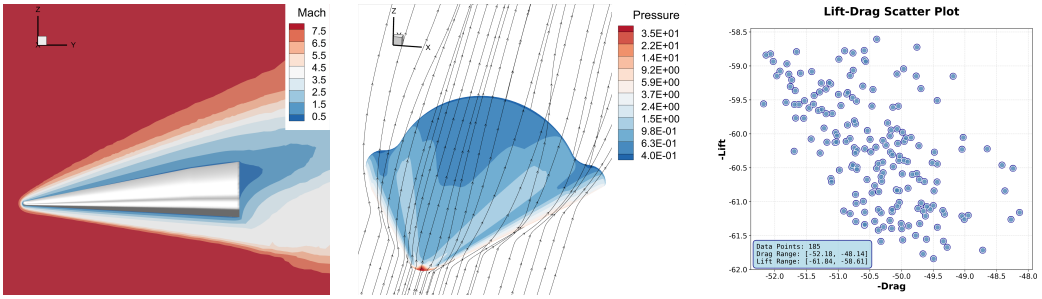


Fig. 2. Hypersonic flow at 85km, Ma = 8, $Kn \simeq 0.0018$**: Mach number contour (left), surface pressure (center), lift/drag scatter plot of all data points (right).**

ACKNOWLEDGEMENTS

Current research is supported by National Key R&D Program of China (Grant Nos. 2022YFA1004500), National Natural Science Foundation of China (12172316, 92371107), Hong Kong research grant council (16301222, 16208324).

REFERENCES

[1] K. Xu, J.-C. Huang, *Journal of Computational Physics* **229**, 7747–7764 (2010).
[2] Y. Zhu, C. Zhong, K. Xu, *Journal of Computational Physics* **315**, 16–38 (2016).
[3] W. Long, Y. Wei, K. Xu, *Physics of Fluids* **36** (2024), https://doi.org/10.1063/5.0232275.
[4] Y. Zhang, Y. Wei, W. Long, K. Xu, *Computer Physics Communications* **314**, 109684 (2025).

An Adjoint Method for Optimization of RGD

R. Caflisch[1,a)] and Y. Yang[2]

[1]*Courant Institute, NYU, USA*
[2]*Cornell University, USA*

[a)]Corresponding author: rec11@nyu.edu

We present a method for optimization of (approximate) solutions of the Boltzmann equation. Optimization is performed following the Discretize-Then-Optimize (DTO) approach, in which DSMC is the discretization method. Optimization for the DSMC solution is performed using an adjoint method, which is similar to the method of Lagrange multipliers. Score functions are used to control random effects for some steps in DSMC. The resulting adjoint method applies to spatial transport, collisions, and boundary conditions, including periodicity, specular reflection, thermal reflection, and prescribed inflow. The adjoint formulation can be used for gradient-based optimization, sensitivity analysis, and design problems involving rarefied gas dynamics.

Abstract 116

Pore-Scale Rarefaction Effects on Aerodynamic Heating of a Gas-Permeable Textile for Deployable Aeroshells

R. Iida[1,a)], K. Yamada[2], and A. Oyama[2]

[1] *The University of Tokyo, Sagamihara, Kanagawa, 252-5210, Japan*
[2] *Institute of Space and Astronautical Science, JAXA, Sagamihara, Kanagawa, 252-5210, Japan*

[a)] Corresponding author: reo-iida@g.ecc.u-tokyo.ac.jp

Deployable flexible aeroshells have emerged as a promising atmospheric entry technology because their lightweight, large-area configuration enables early deceleration in rarefied high-altitude flow regimes, thereby reducing aerodynamic heating. Several flight demonstrations have been conducted [1,2], and applications to Mars entry and Earth reentry from low Earth orbit are under active investigation.

The membrane of demonstrated aeroshell systems is composed of a woven textile, LZY0160W (Toyobo Co., Ltd.), which contains microscopic rectangular pores with characteristic dimensions of approximately 0.1 mm, as shown in Fig. 1. Although such pore structures are intrinsic to woven membranes, their effects on aerodynamic heating during hypersonic entry remain poorly understood. Previous hypersonic wind-tunnel experiments have reported higher heat flux on woven aeroshell models than on impermeable counterparts.

In this study, pore-scale rarefaction effects on aerodynamic heating are investigated across varying Knudsen numbers using computational fluid dynamics (FaSTAR [3], JAXA) and the direct simulation Monte Carlo method (dsmcFoam [4], OpenFOAM). Figure 2 presents representative CFD results for two geometries: a 2-mm-diameter porous region extracted from Fig. 1 (Grid) and an impermeable flat plate of identical diameter (Plain). Under hypersonic wind-tunnel conditions, localized heat flux enhancement is observed near pore edges. The ratio of the surface-integrated heat flux of Grid to that of Plain is 1.22, defined over the same 2-mm projected area under identical freestream and wall boundary conditions, indicating overall heating augmentation due to the porous structure. The augmentation factor decreases with increasing Knudsen number. DSMC simulations confirm this Kn-dependent trend.

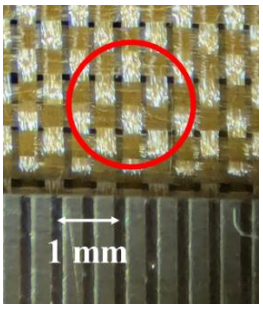


Fig. 1. Micro pores of the aeroshell membrane.

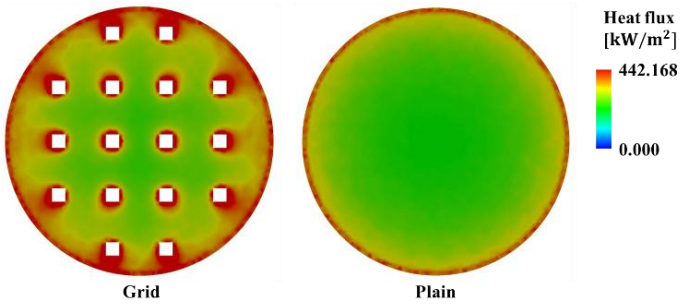


Fig. 2. Heat flux distribution of 2-mm-diameter model with and without 0.1-mm rectangular pores under hypersonic wind-tunnel conditions.

REFERENCES

[1] YAMADA, K., NAGATA, Y., and NAKAO, T., Flight Data Analysis of Reentry Capsule with Deployable Aeroshell in Sounding Rocket S-520-31 Experiment, Proc. of the 26th AIAA Aerodynamic Decelerator Systems Technology Conference (AIAA, 2022), AIAA Paper 2022-2712.
[2] NAGATA, Y., YAMADA, K., NAKAO, T., and HAMORI, H., Suborbital Reentry Flight Demonstration for 2.5 m Deployable Inflatable Flexible Aeroshell Using Sounding Rocket, Journal of Spacecraft and Rockets, 62, pp. 1–12 (2025).
[3] HASHIMOTO, A., MURAKAMI, K., AOYAMA, T., ISHIKO, K., HISHIDA, M., SAKASHITA, M., and LAHUR, P., Toward the Fastest Unstructured CFD Code “FaSTAR”, Proc. of the AIAA 50th Aerospace Sciences Meeting (AIAA, Nashville, TN, 2012), AIAA Paper 2012-1075.
[4] SCANLON, T. J., ROOHI, E., WHITE, C., DARBANDI, M., and REESE, J. M., An Open Source, Parallel DSMC Code for Rarefied Gas Flows in Arbitrary Geometries, Computers & Fluids, 39, pp. 2078–2089 (2010).

Abstract 117

A Multi-level Implicit Discrete Velocity Method to Solve the Relaxation-type Boltzmann Equation

K. Guan[1,a)], and T. Yamada[1,2]

[1] *Graduate School of Engineering, The University of Tokyo, Yayoi 2-11-16, Tokyo, Japan.*
[2] *Institute of Engineering Innovation, The University of Tokyo, Yayoi 2-11-16, Tokyo, Japan.*

[a)] Corresponding author: k-guan@g.ecc.u-tokyo.ac.jp

In this work, we propose a multi-level implicit scheme for the discrete velocity method (DVM) so that the steady state of relaxation-type approximations of the Boltzmann equation can be found with much fewer iterations compared to the conventional counterparts.

We start with the observation that in DVM, finding the steady state is equivalent to finding the solution to a large algebraic system saying that the discrete representation of the flow residual is zero at every physical node. Conventionally this is done using iterative methods (like Gauss-Seidel), but the complexity of the collision term makes it difficult to find the Jacobian of the flow residual with respect to the state variable (namely, the discretized velocity distribution function). As a result, a semi-implicit approach is often used, and the rate of convergence decreases when the relaxation time is short.

In a previous study, we found that for relaxation-type approximations of the Boltzmann equation, the Jacobian corresponding to relaxation can be expressed as the product of two low-rank matrices [1]. For a velocity mesh with N_v nodes, the implicit equation at each node can be solved in $O(N_v)$ time using the Woodbury matrix identity, as opposed to a generic solve costing $O(N_v^3)$. However, the implicit DVM using the Woodbury identity still suffers from slow convergence rates when the number of physical nodes is large.

The main issue lies in the fact that iterative methods can quickly reduce the error modes that oscillate frequently across the physical nodes but hardly influence error modes that are relatively smooth in the physical domain. We propose that the node-wise relaxation using Woodbury identity shown in reference [1] can be enhanced by employing a multi-level framework. In each level, a Woodbury sweep reduces the high-frequency error modes. The remaining residual is mapped to a coarser mesh, where it appears less smooth. Solution in the coarser system is then mapped back to the original system to reduce the smooth error modes. Applying this coarsening strategy recursively, all error modes are expected to be reduced quickly, and the steady state can be found with only a few iterations.

The proposed multi-level method is tested in a 1D flow field. Due to the 1D nature of the physical mesh, the flow Jacobian can be written as a block-sparse matrix consisting of $N_x \times N_x$ blocks (where N_x is the number of physical nodes) where each block is $N_v \times N_v$. Most of the blocks are zero, and the non-zero blocks can be written as the sum of a diagonal component and the product of two low-rank matrices. Exploiting the structure of the Jacobian, we label the nodes alternatively as coarse nodes (C nodes) or fine nodes (F nodes). The fine nodes are separated from each other; hence the linear system can be solved trivially at the fine nodes using node-wise Woodbury relaxation. The coarse system is created as the Schur complement. The multi-level algorithm is completed by implementing this process recursively in a V-cycle.

Numerical experiments show that the total number of V-cycles required before convergence is almost a constant that is independent of Knudsen number, the number of physical nodes, or the number of velocity nodes. Note that the Woodbury relaxation at one node costs $O(N_v)$ and at each recursive level of the V-cycle, the system is reduced by a constant factor. Therefore, the total computational cost for one complete V-cycle is $O(N_x N_v)$. The proposed method relies on the fact that relaxation-type approximations of the Boltzmann equation model the collision term using a relaxed velocity distribution derived from a limited number of macroscopic quantities. Therefore, the proposed model is independent of the exact model one chooses. We expect that the proposed method can be generalized to 2D and 3D flow fields and numerical solutions to the relaxation-type Boltzmann equation can be found with linear complexity.

REFERENCES

[1] K. Guan, T. Yamada, *Transactions of the Japan Society for Computational Methods in Engineering,* **25**, pp. 101-107 (2025).

Abstract 119

Multiscale Analysis of Oxygen Transport in Catalyst Layer of Polymer Electrolyte Fuel Cell

H. Sugihara[1, 2], I. Kinefuchi[3], and T. Tokumasu[2, a)]

[1] *Graduate School of Engineering, Tohoku University.*
[2] *Institute of Fluid Science, Tohoku University.*
[3] *Graduate School of Frontier Sciences, The University of Tokyo*

[a)] Corresponding author: tokumasu@ifs.tohoku.ac.jp

Polymer electrolyte fuel cells (PEFCs) are particularly attractive for fuel cell vehicles because of their low operating temperature and rapid startup capability. However, under high current density conditions, voltage losses due to diffusion polarization become significant, primarily caused by the transport resistance of oxygen molecules within the catalyst layer (CL) [1]. Consequently, improving oxygen transport properties in the CL is a critical issue for enhancing PEFC performance and reducing system costs. Nakauchi et al. showed that the scattering behavior of oxygen molecules on the ionomer surface within the CL can be categorized into surface scattering and surface diffusion [2]. In this study, we employ a multiscale modeling framework in which surface diffusion parameters derived from molecular dynamics (MD) simulations of oxygen molecules on ionomer thin films are incorporated into the direct simulation Monte Carlo (DSMC) method. The objective of this study is to quantitatively evaluate the oxygen transport properties in the catalyst layer of a PEFC.

In the MD simulations conducted in this study, the simulation system consists of carbon walls, Nafion, water molecules, and oxygen molecules. The simulation conditions include a two-dimensional periodic boundary condition and a sampling time of 10 ns. For the DSMC method, a three-dimensional structural model was generated from continuous cross-sectional images of a CL sample obtained by a focused ion beam–scanning electron microscope (FIB-SEM). The simulation conditions include a three-dimensional periodic boundary condition, a time step of 1 ps, and a sampling time of 1 μs.

In this study, the behavior of surface diffusion in the DSMC method was modeled by assuming that oxygen molecules colliding with the wall surface are adsorbed for a certain period, migrate isotopically along the surface, and subsequently undergo diffuse reflection. First, MD simulations were performed to define the time constants and surface diffusion coefficients, which characterize the surface residence time and surface migration distance. The surface residence time obeyed an exponential distribution, with its time constant determined to be τ=20.5 ps. In addition, the surface migration distance followed a Rayleigh distribution, and the surface diffusion coefficient was calculated to be Ds=2.40 Å^2/ps. Next, the influence of surface diffusion on oxygen transport properties was evaluated using the DSMC method. The oxygen transport resistance was calculated to be R=5.52 s/m without surface diffusion. When surface diffusion was considered, the transport resistance increased to R=25.5 s/m. These results indicate that the applied surface diffusion model successfully reproduces the experimentally observed tendency that diffusion is suppressed due to energy loss during collisions between oxygen molecules and the ionomer thin film. However, compared with the experimental value of R = 12.1 s/m, the oxygen transport resistance obtained when surface diffusion was considered significantly higher. This suggests that the current surface diffusion model may overestimate the transport resistance caused by collisions with the ionomer thin film. One possible reason for this is that, in the MD simulations, the definition of oxygen molecules residing on the ionomer thin film may not be sufficiently rigorous.

From these results, it was shown that the suppression of oxygen diffusion caused by collisions with the ionomer thin film can be reproduced by incorporating surface diffusion in addition to accounting for intermolecular interactions between oxygen molecules. However, the simulation results still overestimate the experimental values, indicating that further improvement of the surface diffusion modeling approach is required.

ACKNOWLEDGEMENTS

The simulations in this study were performed using the Next-Generation Integrated Research System at the Institute of Fluid Science, Tohoku University. The authors would like to express their sincere gratitude to all those invoices.

REFERENCES

[1] S. J. Peighambardoust, et al., *International Journal of Hydrogen Energy*, **35**, pp.9349–9384 (2010).
[2] M. Nakauchi, et al., *The Journal of Physical Chemistry C*, **123**, pp.7125-7133 (2019).

Propellant Transport Modeling of Atmosphere-Breathing Electric Propulsion Using a DSMC-Centered Numerical Framework

G. Moon[1], M. Yi,[2] and E. Jun[1,a)]

[1]*Korea Advanced Institute of Science and Technology, 34141, Daejeon, Republic of Korea.*
[2]*Agency for Defense Development, 34186, Daejeon, Republic of Korea.*

[a)]Corresponding author: eunji.jun@kaist.ac.kr

Very Low Earth Orbit (VLEO) is typically defined as altitudes below 500 km and offers significant advantages for Earth-observation resolution and reduced satellite launch costs [1]. However, the residual rarefied atmosphere imposes a continuous drag force, rendering propulsion essential for drag-compensation maneuvers. Electric Propulsion (EP) systems have been considered for orbital maintenance in VLEO due to their high specific impulse, yet the necessity for significant onboard propellant mass constrains long-term missions [1]. Atmosphere-Breathing Electric Propulsion (ABEP) offers an alternative solution by capturing ambient atmospheric particles *in situ* for use as propellant [2]. Fig. 1 illustrates the design components and propellant transport schematic of the ABEP system. The propellant gas in ABEP systems undergoes multi-scale and multi-physical processes, including rarefied gas capture, compression, discharge, and plasma plume expansion. Previous studies have conducted extensive numerical investigations on individual components such as intake devices, storage units, and thrusters [3–5]. Nevertheless, these investigations have primarily treated each subsystem in isolation and relied on distinct methodologies and assumptions.

This study performs a sequential analysis of the entire propellant transport process by establishing a consistent numerical framework based on the Direct Simulation Monte Carlo (DSMC) method, enabling the evaluation of the operational feasibility of ABEP in VLEO. To describe the multi-physical behavior of the ABEP propellant, the DSMC-centered framework integrates additional physical modules, including an atmospheric model, a phase-change model, and a collisional plasma solver. Based on this framework, First, the correlation between captured gas kinetics and the geometry of the passive intake device is characterized to derive an optimized intake design. Second, a cryogenic storage system is investigated to enhance the transport and pressurization of the captured gas, and the performance of the intake-storage assembly is estimated. Third, the exhaust plasma plume is analyzed under atmospheric composition and VLEO ambient conditions, focusing on the ion backflow phenomenon and potential spacecraft contamination. Finally, synthesizing the propellant transport characteristics, a system-level assessment of the power balance and drag compensation feasibility is conducted for an ABEP-integrated spacecraft operable in VLEO.

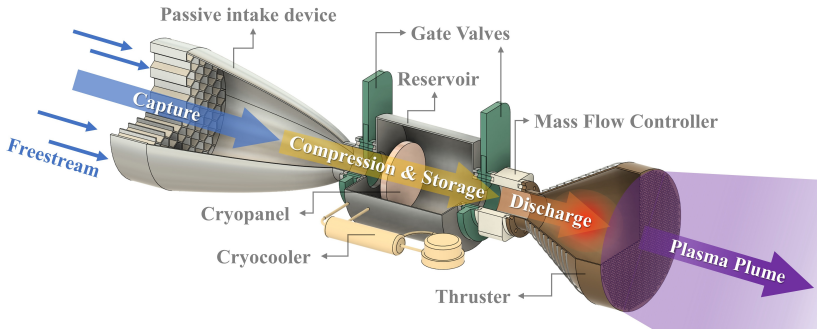


Fig. 1. Schematics of the ABEP design components and propellant transport.

ACKNOWLEDGEMENTS

This work was supported by the Agency for Defense Development of the Korean Government (UG233092TD). This work was supported by the National Supercomputing Center with supercomputing resources including technical support (KSC-2025-CRE-0573).

REFERENCES

[1] S. Fasoulas, A. S. Pagan, C. Traub, B. Annighöfer, S. Barz, A. Beck, T. Cunis, T. Dekorsy, S. Essig, W. Fichter, B. Flemisch, G. Herdrich, T. Hobiger, I. Kallfass, J. Kästner, S. Klinkner, G. Lamanna, S. Loehle, M. Pfeiffer, R. Poser, J. Roth, M. Saliba, M. Schneider, N. Sneeuw, G. Wagner, *CEAS Space Journal* (2025).
[2] G. Moon, M. Yi, K. Park, Y. Kim, H. Yoon, E. Jun, *Vacuum* **212**, 112066 (2023).
[3] T. Andreussi, E. Ferrato, V. Giannetti, *Journal of Electric Propulsion* **1**, 31 (2022).
[4] G. Moon, M. Yi, E. Jun, *Aerospace Science and Technology* **151**, 109300 (2024).
[5] G. Moon, W. Choe, E. Jun, *Plasma Sources Science and Technology* **32**, 125012 (2023).

Development of ab initio-based chemistry model for atmospheric entry into Jupiter

Devendra Koushal[1,a)], Tapan K. Mankodi[2] and U. V. Bhandarkar[1]

[1]*Indian Institute of Technology Bombay, India.*
[2]*Indian Institute of Technology Guwahati, India.*

[a)]Corresponding author: devendrakoushal567@gmail.com

Future Jovian missions require accurate predictions of thermal load during atmospheric entry, where the extreme hypersonic speed of probe generates a strong non-equilibrium flow. In the present work, DSMC method has been employed to simulate the Jovian atmospheric entry. During extreme entry conditions, the phenomenological reaction model may fail, therefore an *ab initio*-based reaction model has been developed and integrated in direct simulation Monte Carlo (DSMC) [1, 2] method. . Collision induced dissociation cross-section (CID) for three different reactions (H_2 + H, H_2 + He, and H_2 + H_2) has been calculated using the quasi classical trajectory (QCT) [3] method. Simulations are performed at two different altitudes of Jupiter's atmosphere. At each altitude, two separate simulations are performed: one using the conventional total collision energy (TCE) model and the other using an *ab initio*–based reaction model. A comparison of species mole fraction profile and the different modes of temperatures using TCE and *ab initio*-based reaction model has been shown. Fig. 1 presents a comparison of the translational temperature and pressure contour obtained using the TCE model and the *ab initio*–based reaction model. The results indicate that the DSMC method using *ab initio*–based model predicts a higher translational temperature compare to the TCE model.

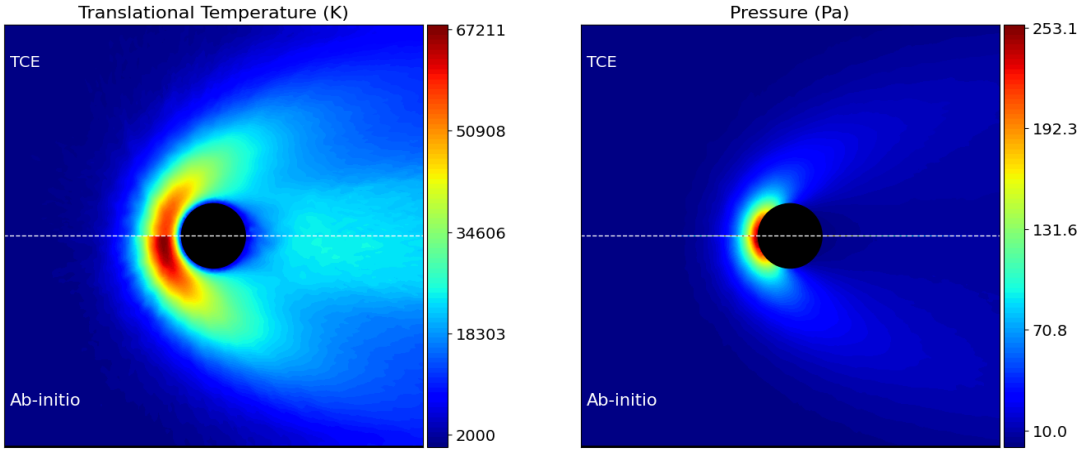


Fig. 1 Comparison of translational temperature and pressure using TCE and *ab initio*-based reaction model

REFERENCES

[1] G. A. Bird. Monte carlo simulation of gas flows. *Annual Review of Fluid Mechanics*, 10:11–31, 1978.
[2] G. A. Bird. *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*. Oxford Science Publications, New York, 1994.
[3] M. Karplus, R. N. Porter, and R. D. Sharma. Exchange reactions with activation energy. i. simple barrier potential for (h, h_2). *Journal of Chemical Physics*, 43:3259–3287, 1965.

Abstract 122

DSMC-CFD Consistency in the Continuum/Transition Overlap Region for a Deployable Mars Capsule

F. Portis[1,a)], D. D'Ambrosio[1], and A. Schettino[2]

[1] *Politecnico di Torino, Corso Duca degli Abruzzi, 24, 10129 Torino, Italy.*
[2] *Italian Aerospace Research Centre (CIRA), Via Maiorise, 81043 Capua, Italy.*

[a)] Corresponding author: federica.portis@polito.it

Atmospheric re-entry is a critical phase for any space mission. To accurately model the flowfield around a vehicle during re-entry, it is essential to identify the flow regimes encountered along the trajectory. The re-entry of a hypersonic vehicle begins in an extremely rarefied environment, where the particle number density is low and the mean free path is large. As a result, the Knudsen number (Kn), defined as the ratio of the mean free path (λ) to a characteristic length (D), exceeds the limit of 10, corresponding to the Free Molecular Flow (FMF) regime. Under these conditions, the classical governing equations of fluid dynamics, i.e., the Navier–Stokes (N-S) equations, fail to capture the physics because the continuum hypothesis breaks down. Therefore, a different approach is required: the Direct Simulation Monte Carlo (DSMC) method, which is based on the Boltzmann equation. DSMC analyses can be extended to the transition regime (0.01<Kn<10), where the particle density increases and the mean free path decreases, driving the Knudsen number toward the continuum limit ($Kn \approx 0.01$).

In the overlap between the transition and continuum regimes, DSMC can still be applied. However, as the number of simulated particles increases, the computational cost grows dramatically. Although the underlying physics allows DSMC analyses to extend into the continuum regime, the associated computational cost makes its use in the fully continuum regime prohibitive. Conversely, continuum Computational Fluid Dynamics (CFD) solvers based on the Navier-Stokes equations perform well when the continuum hypothesis holds, but their validity becomes questionable as the flow approaches the transition regime. To extend the validity of N-S based methods, slip boundary conditions are implemented [1]. These conditions allow N-S-based methods to capture the flow physics more accurately for Knudsen numbers slightly above 0.01. Consequently, an overlap region exists in which both DSMC and continuum CFD solvers are applicable, and consistency between the two approaches must be ensured.

The DSMC simulations in this work are performed using the SPARTA code [2], with a Variable Hard Sphere (VHS) collision model and a Total Collision Energy (TCE) chemistry model following the reactions described by Park et al. [3]. The CFD simulations are carried out using the commercial solver STAR-CCM+ and include chemical reactions consistent with the DSMC setup, transport properties from Gupta et al. [4], and thermodynamic properties based on NASA polynomials. The 2D analyses consider a deployable capsule in the Mars atmosphere, building upon the results of Portis et al. [5].

This work aims to improve the consistency between DSMC and continuum CFD by tailoring the CFD model so that transport properties and chemical kinetics are aligned with those used in the DSMC simulations.

ACKNOWLEDGEMENTS

This publication is part of the project PNRR-NGEU which has received funding from the MUR – DM 117/2023 and is co-funded by C.I.R.A.

REFERENCES

[1] T. Gokcen, R. MacCormack, D. Chapman, Computational fluid dynamics near the continuum limit, *Proc. of the 8th Computational Fluid Dynamics Conference* (Honolulu, 1987).
[2] S. J. Plimpton, S. G. Moore, A. Borner, A. K. Stagg, T. P. Koehler, J. R. Torczynski, M. A. Gallis, Direct Simulation Monte Carlo on petaflop supercomputers and beyond, Physics of Fluids, **31,** 086101 (2019).
[3] C. Park, J. T. Howe, R. L. Jaffe, and G. V. Candler, Review of Chemical-Kinetic Problems of Future NASA Missions, II: Mars Entries, Journal of Thermophysics and Heat Transfer, Vol. **8**, No.1 (1994).
[4] R. N. Gupta, J. M. Yos, R. A. Thompson, A review of reaction rates and thermodynamic and transport properties for an 11-species air model for chemical and thermal nonequilibrium calculations to 30000 K, NASA Technical Memorandum 101528 (1989).
[5] F. Portis, D. D'Ambrosio, T. E. Schwartzentruber, P. Vernillo, A. Schettino, Comparison between CFD and DSMC Analysis for a Deployable Mars Entry Vehicle, *Proc. of the DSMC 2025 conference* (Santa Fe, 2025).

Kinetic Modelling of Rarefied Gas Flows with Radiation

Q. Li[1,a)], J. Zeng[2] and L. Wu[2]

[1]*Sun Yat-sen University, China*
[2]*Southern University of Science and Technology, China*

[a)]Corresponding author: liqi99@mail.sysu.edu.cn

Space exploration missions involve spacecraft entering planetary atmospheres at hypervelocity, generating extreme aerothermal environments. Radiative heat flux can constitute a significant or even dominant portion of the total thermal load under these conditions. The coupling between radiation effects and strongly non-equilibrium rarefied gas flows presents a critical challenge for thermal protection system design, and severely impacts aerothermal optical measurements. Current numerical approaches typically incorporate radiative transport macroscopic fluid equations, which fail to capture strong non-equilibrium effects. Alternatively, bidirectional coupling between the Direct Simulation Monte Carlo method and the Photon Monte Carlo method suffers from statistical noise, leading to stability issues in coupled field solutions.

This work develops a kinetic model for high-temperature rarefied gas flows with bound-bound radiation, induced by transitions between excited internal energy levels (e.g., vibrational, electronic) of gas molecules. For high-temperature electronic excitation and radiation, our kinetic model accurately captures both the transport coefficients and the underlying relaxation processes, such as the internal energy exchange caused by heavy-particle impacts. This ensures its consistency with state-to-state approaches in the continuum limit. The non-equilibrium dynamics of gas flow and radiation are tightly coupled, where the transport properties of gas molecules and photons are correlatively dependent. The radiation spectrum can be obtained by incorporating the gasˇ2013photon interaction at each internal energy level and considering the frequency-dependent transition probability and photon intensity. For vibrational excitation and radiation, the model employs the reductions of the mesoscopic distribution function combined with intra-modal equilibrium assumptions to efficiently simulate radiative heating from vibrational transitions in rarefied gases. Finally, a multiscale algorithm for coupled flow-radiation fields is developed based on the general synthetic iterative scheme. This approach permits computational grids much larger than the molecular and photon mean free path, and achieves converged solutions within a hundred iterations in all flow regimes, enabling asymptotic-preserving and fast convergence modeling of radiative gas flows.

References

[1] Q. Li, J. Zeng, Z. Huang, L. Wu, Kinetic modelling of rarefied gas flows with radiation, Journal of Fluid Mechanics 965 (2023) A13

[2] J. Zeng, Q. Li, Y. Zhang, W. Su, L. Wu, Accelerated simulation of multiscale gas-radiation coupling flows via a general synthetic iterative scheme, under review, (2026)

Variance Reduction in the Fokker–Planck Particle Method for Rarefied Gases using Quasi-Random Numbers

L. Netterdon[1,a)], V. Montanaro[2], H. Gorji[3] and M. Torrilhon[1]

[1]*RWTH Aachen University, Germany*
[2]*École Polytechnique Fédérale de Lausanne, France*
[3]*Swiss Federal Institute of Material Sciences*

[a)]Corresponding author: netterdon@acom.rwth-aachen.de

The Fokker–Planck (FP) particle method accelerates rarefied-gas simulations by replacing the binary collisions of the commonly used Direct Simulation Monte Carlo (DSMC) method with a drift–diffusion process. The drift and diffusion coefficients are constructed so that the gas relaxes toward the correct equilibrium, the H-theorem is satisfied, and relevant moments decay at the proper rates. As in all particle methods, statistical noise leads to fluctuations in macroscopic quantities and therefore requires large particle numbers to achieve accurate estimates.

This presentation investigates the use of quasi-random numbers, which cover distributions more evenly than pseudo-random numbers and thereby reduce estimator variance. To preserve this advantage across time steps, an Array Randomized Quasi-Monte Carlo (Array-RQMC) strategy is applied, ensuring that particles close in velocity space are advanced with consecutive elements of the quasi-random sequence. The resulting FP–Array-RQMC method is evaluated for homogeneous and inhomogeneous problems and compared with established variance-reduction approaches. Numerical results demonstrate improved convergence rates and substantially smaller errors for sufficiently large particle numbers.

Numerical characterisation of a supersonic bidirectional vortex inductively coupled plasma torch

L. Riou[1,2,a)], A. Bilocq[3], D. Henneaux[3], P. Schrooyen[2], K. Hillewaert[2,3,4], T. Magin[2,5] and T. Lafleur[1]

[1]*School of Engineering and Technology, University of New South Wales Canberra, Canberra, Australia*
[2]*Aeronautics and Aerospace Department, von Karman Institute for Fluid Dynamics, Sint-Genesius-Rode, Belgium*
[3]*Cenaero, Gosselies, Belgium*
[4]*Department of Aerospace and Mechanical Engineering, Université de Liège, Liège, Belgium*
[5]*Aero-Thermo-Mechanics Department, Université Libre de Bruxelles, Bruxelles, Belgium*

[a)]Corresponding author: landry.riou@unsw.edu.au

Radio-Frequency (RF) Inductively Coupled Plasma (ICP) torches were introduced in the early 1960s as thermal plasma generators. They consist of a hollow dielectric tube around which an RF coil is wrapped. Gas is injected from one end of the tube while the opposite end is either open or attached to a nozzle. A plasma discharge is created by the inductive RF fields and the resulting high-temperature, high-purity (as the discharge is electrodeless) gas, as well as the possibility to generate a supersonic flow with a convergent-divergent nozzle, makes them suitable for a wide range of engineering applications such as gas conversion and pyrolysis, nano-powder spheroidisation and formation, material processing, material testing for reentry applications, and space propulsion. Currently, conductive heat losses to the tube walls is one of the main power inefficiency mechanisms in supersonic ICPs [1]. An innovative gas injection configuration, named the bidirectional (or reverse) vortex (see Fig. 1), and first introduced for subsonic ICPs by Gutsol *et al.* [2], has recently been revisited for supersonic ICPs [3] showing a strong increase in thermal efficiency compared to conventional gas injection configurations. However, due to experimental limitations, the interaction between the bidirectional vortex flow field, the plasma discharge, and the supersonic nozzle has yet to be understood. In this work, we use a steady 2D-axisymmetric self-consistent MagnetoHydroDynamic (MHD) model with swirl to characterise a supersonic bidirectional vortex inductively coupled plasma torch. The model is discretised using the high-order multi-domain Discontinuous Galerkin method in Cenaero's massively parallel multi-physics platform Argo, with thermodynamic and transport properties computed using the Mutation++ library [4]. Preliminary results suggest that the bidirectional vortex can be prevented from reaching the upstream end of the chamber at high powers and/or low mass flow rates, while a strong increase in the swirl velocity is seen near the nozzle throat region due to conservation of flow angular momentum.

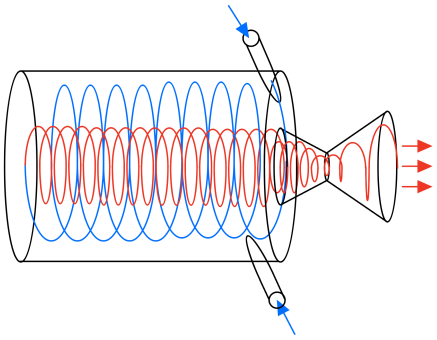


Fig. 1. Schematic of a supersonic bidirectional vortex inductively coupled plasma torch. The RF coil is omitted for clarity.

ACKNOWLEDGEMENTS

This material is based upon work supported by the Air Force Office of Scientific Research under award number FA2386-24-1-4004.

REFERENCES

[1] T. Lafleur, C. S. Corr, *Journal of Applied Physics* **130**, 043304July (2021).
[2] A. Gutsol, J. Larjo, R. Hernberg, *Plasma chemistry and plasma processing* **22**, 351–369 (2002).
[3] A. Pascale, T. Lafleur, C. S. Corr, *Journal of Physics D: Applied Physics* **56**, 105202March (2023).
[4] J. B. Scoggins, V. Leroy, G. Bellas-Chatzigeorgis, B. Dias, T. E. Magin, *SoftwareX* **12**, 100575July (2020).

Chemiluminescence-Based Investigation of Methane Flame Gas–Surface Interactions and TPS Ablation via Propane-Fueled HVOF Experiments

Deog Gyun Cho[1], Jong Geun Bae[1], Se Youn Moon[1,2]

[1]High-enthalpy Plasma Research Center, [2]Dept. Quantum System Engineering, Jeonbuk Nat'l Univ., Republic of Korea

Gas–surface interaction in high-enthalpy reacting flows governs the ablation behavior of thermal protection system (TPS) materials during hypersonic flight and atmospheric entry. Methane is increasingly adopted as a next-generation aerospace fuel; however, experimental datasets describing TPS ablation under methane-based reacting flows remain limited due to the difficulty of reproducing such environments in ground-test facilities. To address this limitation, this study presents an extrapolative experimental–modeling framework that derives methane-flame gas–surface interaction behavior using existing propane-fueld high-velocity oxy-fuel (HVOF) experimental data.

Although HVOF systems operate with propane rather than methane, both fuels generate key combustion intermediates—CH, OH, and C_2 radicals—that govern heat release, oxidation potential, and near-wall chemical processes. In this work, propane-fueled HVOF flames are treated as methane-analog reactive flows, and time-resolved diagnostics are used to develop physics-based scaling relationships applicable to methane environments. Flame heat flux and temperature are measured using heat-flux gauges and thermocouples, while high-speed imaging and optical displacement techniques quantify transient surface recession and morphological evolution of carbon-based TPS materials.

Simultaneously, chemiluminescence imaging of electronically excited OH, CH, and C_2 radicals are employed as a non-intrusive diagnostic to resolve flame structure, reaction-zone dynamics, and near-surface chemical activity. The spatial and temporal evolution of radical emissions is correlated with measured ablation rates, revealing strong coupling between gas-phase reaction dynamics, localized heat-release fluctuations, and oxidation-driven surface recession. Variations in OH, CH, and C_2 emission intensities provide insight into methane-relevant ablation behaviors, including reduced soot-related shielding and enhanced oxidation dominance.

The experimentally derived heat-flux histories, temperature distributions, and chemiluminescence-informed combustion characteristics are incorporated into coupled reacting-flow and material-response modeling to extrapolate TPS ablation behavior under methane-flame conditions. This approach provides a physically grounded pathway for predicting methane-flame gas–surface interaction in the absence of direct experimental data, supporting improved

model validation and TPS design for future methane-fueled hypersonic and atmospheric-entry applications.

Keywords: Gas–surface interaction, Thermal protection systems (TPS), Ablation modeling, Chemiluminescence diagnostics, Methane-analog combustion (propane HVOF)

Molecular Beam-Surface Scattering Dynamics Relevant to Satellites in Very Low Earth Orbit (VLEO)

Timothy K. Minton,[1,a)] Pedro D. C. Jorge,[1] Chenbiao Xu,[1] Celeste H. Guiles[1]

[1] *Smead Dept. of Aerospace Engineering Sciences, Univ. of Colorado, Boulder, CO, USA*

[a)] Corresponding author: tminton@colorado.edu

There is an explosion of interest in the utilization of very low Earth orbit (VLEO, roughly 100 – 350 km altitude) for commercial and military purposes. Despite the obvious proximity advantages of VLEO, these altitudes have long been avoided because of the high density and harsh oxidizing environment of the residual atmosphere, which contains atomic oxygen (AO) and molecular nitrogen (N_2). Momentum exchange in collisions between these species and satellite surfaces results in aerodynamic drag. Aside from drag, materials on the external surfaces of VLEO satellites may react chemically with AO, resulting in oxidation, erosion, roughening, and degradation of function. Minimizing and predicting drag and maximizing AO resistance are crucial for proliferated VLEO operation. We have used molecular beams of O and O_2, traveling at orbital velocities of ~8 km s^{-1}, to investigate both the AO resistance and drag potential of various materials that may be used on VLEO satellites. The pulsed molecular beam, produced from a laser-driven breakdown source, was used to expose selected materials to AO fluences up to ~1×10^{21} O atoms cm^{-2}. Some of these materials were also exposed to the LEO environment on the International Space Station to similar AO fluences. Materials that exhibited significant AO resistance were used in molecular beam-surface scattering experiments, and the scattering dynamics were measured as a function of both polar (θ) and azimuthal (ϕ) scattering angles on pristine and pre-exposed sample surfaces. Additional experiments were conducted with near orbital-velocity Ar and O atoms on six different deliberately roughened Kapton polyimide surfaces to explore the relationship between surface roughness and scattering dynamics (Fig. 1). The velocity and angular distributions of scattered O and Ar atoms depend strongly on the incident angle of the impinging atoms and the roughness of the surface in ways that are not *a priori* predictable. Nevertheless, trends are emerging that point the way to low-drag and AO-resistant material surfaces that have potential for use on VLEO satellites. Based on the scattering dynamics data, gas-surface scattering models have been formulated, allowing for the calculation of overall energy and momentum accommodation and for simulations of satellite drag.

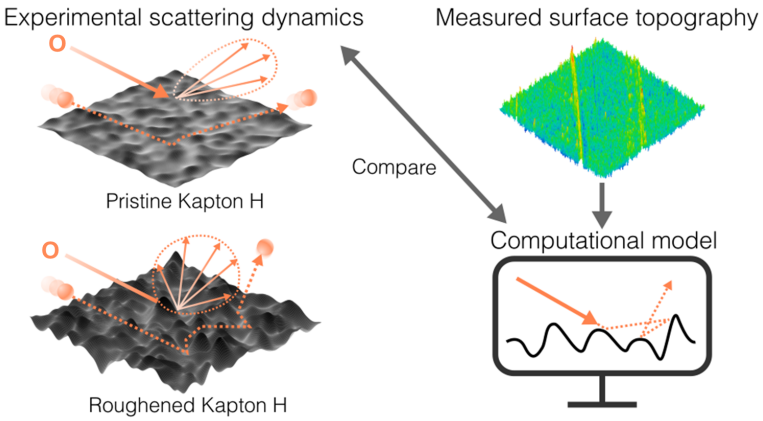


Fig. 1. Illustration of O-atom inelastic scattering on a pristine and roughened Kapton H surface. The scattering dynamics become increasingly diffuse as the surface roughness increases. A model, combining gamma-distributed surfaces for geometrical roughness and a CL local scattering kernel was used to fit the experimental scattering data. The fitted roughness parameters correlated positively with topographical parameters measured by atomic force microscopy, although they did not match these parameters directly.

ACKNOWLEDGEMENTS

This work has been supported by the U.S. Air Force Office of Scientific Research (FA9550-23-1-0162), the U.S. Defense Advanced Research Projects Agency (Cooperative Agreement No. HR0011-25-2-0008), and the Nanyang Technological University (AWD-24-09-0026).

LIF Measurements and Hybrid Modeling of Transitional Flow in a High-Flux Campargue-Type Rb Atomic Beam Source

K. Chandrasekar[1,a)] and C. M. Limbach[1]

[1] *University of Michigan, Ann Arbor, MI, 48109*

[a)] Corresponding author: kaeshavc@umich.edu

Recent studies have demonstrated that optomechanical coupling between co-propagating laser and atomic beams can produce a self-guiding effect, wherein the atomic beam induces refractive guiding of the laser while the laser confines the atoms through optical dipole forces [1–3]. The stability and performance of such coupled beams depend critically on the atomic beam number density and translational temperature. These requirements motivate the use of high pressure-ratio supersonic expansions rather than effusive sources commonly employed in cold-atom experiments.

To achieve the required beam properties, a Campargue-type source configuration was selected, as shown in Fig. 1. This combines a supersonic expansion stage with a downstream skimmer that isolates the high-density, low-temperature core of the jet [4]. Prior studies have focused on the pre-skimmer free expansion region, where stagnation-to-ambient pressure ratios ($\eta > 100$) produce extreme cooling and acceleration of the flow [5]. In contrast, the post-skimmer region, where beam transport and future laser Doppler cooling will occur, remains under-characterized in density profile, velocity spread, and source geometry dependence, limiting predictive control of self-guiding.

The present work investigates the geometric and gasdynamic influences, particularly nozzle-skimmer geometries and pressure ratio, governing post-skimmer flow conditions. Laser-induced fluorescence (LIF) measurements are performed in noble-gas flows seeded with atomic rubidium to obtain spatial density profiles and velocity distribution functions downstream of the skimmer. To complement the experimental effort, a computationally efficient reduced-order modeling framework is developed to enable rapid prediction and design iteration. The continuum-to-rarefied transition is treated using a staged approach consisting of (1) method-of-characteristics (MOC) simulation of the free jet expansion, (2) application of the sudden-freeze approximation, and (3) solution of the collisionless gas-kinetic equations in the downstream region. The resulting novel framework, extending the results of MOC simulations to free molecular flow, supports rapid design optimization and is benchmarked against LIF measurements.

These results provide design guidance for producing dense, cold atomic beams relevant to optomechanical coupling, fundamental light-matter interaction studies, and emerging in-space beamed power and propulsion concepts.

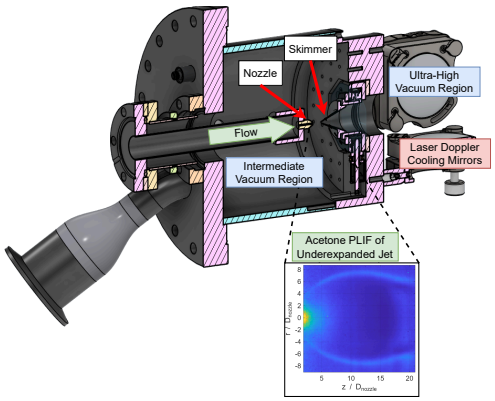


Fig. 1. Labeled Campargue-type beam source design cross-section with an underexpanded jet image.

ACKNOWLEDGEMENTS

The authors would like to thank the National Aeronautics and Space Administration for support of the first author by a NASA Space Technology Graduate Research Opportunity (Grant No. 80NSSC24K1335).

REFERENCES

[1] C. M. Limbach, H. P. Morgan, *Acta Astronautica* (2022).
[2] K. Chandrasekar, C. M. Limbach, *AIAA Aviation Forum and ASCEND* (2025).
[3] A. Jewell, Y. Bao, C. M. Limbach, *AIAA SciTech Forum* (2026).
[4] R. Campargue, *J. Phys. Chem.* **88**, 4466–4474 (1984).
[5] K. Chandrasekar, C. M. Limbach, *AIAA SciTech Forum* (2026).

Model of Thermal Slip Under Near-Wall Fluid-Solid Interaction Potentials

T. Tsuji[1,a)], K. Takita,[1] and S. Taguchi[1]

[1] *Graduate School of Informatics, Kyoto University, Kyoto, Japan.*

[a)] Corresponding author: tsuji.tetsuro.7x@kyoto-u.ac.jp

Gas flows induced by inhomogeneous wall temperature profiles are referred to as thermal transpiration. This thermally-induced flow stems from molecular-scale non-equilibrium effects and is thereby expected to find applications in small scale systems and/or low pressure environments, where the molecular mean free path is comparable to the characteristic flow length. In particular, thermal transpiration has been considered important in the development of motionless heat-driven pumping systems, such as Knudsen pumps, and in the understanding of the driving mechanism of thermophoresis, particle motion in an inhomogeneous temperature profile of fluids.

In liquids, a similar type of thermally-induced flow has been reported in the literature, often referred to as thermo-osmosis. Recent experiments [1] and molecular simulations [2, 3] on thermo-osmosis in nanoscale fluid systems have shown that molecular scale effects, such as the properties of fluid-solid interfaces, make a significant contribution to flow characteristics. From a macroscopic view point, thermal transpiration and thermo-osmosis can be described as velocity slip on the wall surface induced by inhomogeneous temperature distribution, namely, thermal slip. Therefore, the modeling of thermal slip incorporating fluid-solid molecular interaction is useful for understanding the mechanism of thermally-induced flows and to develop applications. In this presentation, we report the development of a slip-flow theory for rarefied gases accounting for the effect of near-wall fluid-solid interaction potential [4]. We find that, despite differences in the molecular-scale descriptions of gases and liquids, the effects of the interaction potential characteristics show similar trends: favorable (or unfavorable) interactions tend to drive the slip flow from the cold side to the hot side (or vice versa).

We briefly describe a physical model as follows. We consider a gas confined between two parallel plates with a linear wall-temperature profile, such as a standard thermal-transpiration configuration (e.g. Ref. [5]). The gas behavior is described by the Bhatnagar–Gross–Krook (BGK) model of the Boltzmann equation. The boundary condition of the BGK model on the surfaces of the plates is the diffuse-reflection boundary condition. Near-wall interaction potentials are prescribed between the gas molecules and the plates, exerting wall-normal forces on the gas molecules. The temperature gradient along the plates is sufficiently small so that the system can be linearized around a non-uniform reference equilibrium state under the near-wall potential. We apply the generalized slip-flow theory [6] to obtain a thermal-slip boundary condition for this system. We find that, under the scaling assumption that the effective range of the potential is on the same order as the mean free path, the slip-flow theory works as in the case where the potential is absent. The results of the slip-flow theory well reproduce the computational results from a direct numerical analysis of the same problem. When a purely-attractive potential is prescribed, the thermal slip directed from the cold side to the hot side is enhanced, while a purely-repulsive potential reduces the magnitude of thermal slip and can even reverse the flow direction at sufficiently large potential strength. Such flow reversal is qualitatively consistent with previous molecular simulations [2, 3].

ACKNOWLEDGEMENTS

This work was supported by the Japan Society for the Promotion of Science KAKENHI Grants No. 22K18770, No. 22K03924, No. 24K00803, and No. 25K01156 and also by the Japan Science and Technology Agency PRESTO Grant No. JPMJPR22O7.

REFERENCES

[1] A. P. Bregulla, A. Würger, K. Günther, M. Mertig, F. Cichos, *Physical Review Letters* **116**, 188303 (2016).
[2] L. Fu, S. Merabia, L. Joly, *Physical Review Letters* **119**, 214501 (2017).
[3] P. Anzini, Z. Filiberti, A. Parola, *The Journal of Chemical Physics* **162**, 094501 (2025).
[4] T. Tsuji, K. Takita, S. Taguchi, *Physical Review Fluids* **10**, 114202 (2025).
[5] T. Ohwada, Y. Sone, K. Aoki, *Physics of Fluids* **1**, 2042–2049 (1989).
[6] Y. Sone, *Molecular Gas Dynamics: Theory, Techniques, and Applications* (Birkhäuser Boston, 2007).

A flow field for studying recombination and vibrational de-excitation rates

H. G. Hornung[1,a)], J. M. Austin,[1], R. G. Watt,[2], P. A. Jacobs,[2] and R. J. Gollan[2]

[1]*California Institute of Technology, Pasadena, CA91125, USA.*
[2]*The University of Queensland, St. Lucia, Qld 4067, Australia*

[a)]Corresponding author: hghornung@gmail.com

The dissociation and vibrational excitation rates needed for high-speed non-equilibrium gas dynamics are usually measured in shock tubes, because a shock wave provides a suitable sudden change in conditions for the gas to respond to. However, recombination and vibrational de-excitation rates are not as easy to measure directly, so that they are usually determined by setting them equal and opposite to the dissociation and excitation rates at equilibrium. A suitable flow field to study the backward rates directly is the expansion around a convex corner. The state upstream of the expansion should be a uniform highly excited and dissociated equilibrium state, such as may be generated by the plane oblique shock on a wedge just below the detachment angle. In an expansion following this state the rate of change of conditions imposed on the gas along streamlines decreases with the distance of the streamline from the corner thus providing a rich field for studying backward rates. In preparation for planned spectroscopic measurements in the T5 shock tunnel we explored such a flow by using the Eilmer software system of UQ [1]. Specifically, we used the four-temperature air model with Modified Marrone-Treanor (MMT) [2] and Park [3] reaction rates. Because the experiment will be with a wedge of finite span, and the methods to be used are line-of-sight integrating, both 2D and 3D computations were made.

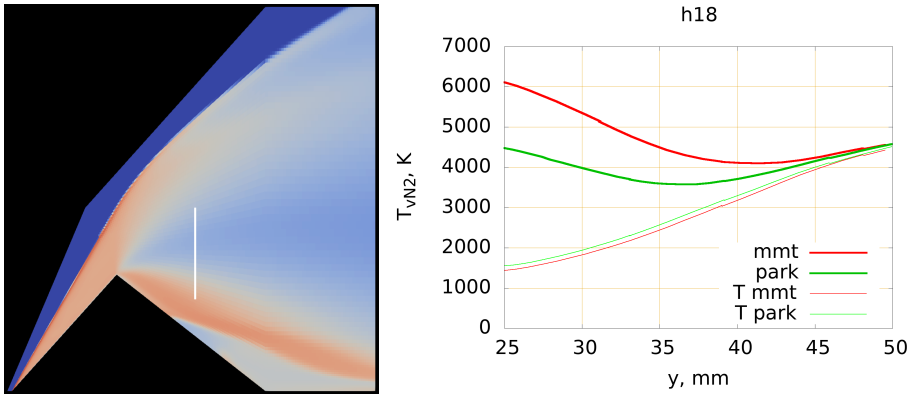


Fig. 1. LEFT: Distribution of vibrational temperature of N2. RIGHT: Distribution of vibrational and translational (faint) temperature along the white line in the left figure according to MMT and Park rates.

Fig. 1 shows an example of the results in the case of flow at 18 MJ/kg. The color map shows the vibrational temperature of N2, also displaying a white line along which the graph shows the distribution of vibrational and translational temperatures. It clearly indicates that at the lower end of the white line, the flow is very far from equilibrium, while it has almost reached equilibrium at the upper end of the line. It also shows large differences between the two models.

ACKNOWLEDGEMENTS

This work was supported in part by the Air Force Office of Scientific Research through AFOSR grant number FA9550-23-1-0446.

REFERENCES

[1] N. N. Gibbons, K. A. Damm, P. A. Jacobs, R. J. Gollan, *Comp. Phys. Comm.,* **282(108551** (2023).
[2] R. S. Chaudry, I. D. Bird, E. Torres, T. E. Schwartzentruber, G. V. Candler, *AIAA* **Paper 2020-2191** (2020).
[3] C. Park, *J. Thermophys. and Heat Transfer* **7**, 385–429 (1993).

Accurate PIC Simulation of Ion Optics using p-Adaptation on Tetrahedral Meshes

K.-S. Ellenberger[a)], **T. Ott**,[b)], S. Fasoulas, and M. Pfeiffer

Institute of Space Systems (IRS), University of Stuttgart, Pfaffenwaldring 29, 70569 Stuttgart

[a)]Corresponding author: ellenbergerk@irs.uni-stuttgart.de
[b)]Corresponding author: ottt@irs.uni-stuttgart.de

Accurate numerical simulations of the experimental setup are essential for the design and optimization of ion optics. Particle-in-cell (PIC) methods are widely used for this purpose, as they allow a self-consistent treatment of charged particle dynamics and electromagnetic fields. However, the complex geometrical structures typically present in ion optical setups pose significant challenges for mesh generation and numerical efficiency.

In particular, the use of structured hexahedral meshes becomes problematic for geometries featuring intricate electrodes, curved surfaces, and narrow gaps. These limitations can lead to poor mesh quality, reduced numerical accuracy, or excessive computational cost due to mesh refinement algorithms. To address this issue, the present work investigates the use of unstructured tetrahedral meshes as an alternative strategy for PIC simulations of ion optics with the open-source software PICLas [1, 2].

A workflow based on tetrahedral mesh elements is described to robustly represent complex beamline geometries while maintaining sufficient resolution in critical regions. To further improve computational efficiency, the field solver is formulated using a continuous Galerkin (CG) method. In addition, a p-adaptation strategy is explored, supporting a variable, element-local polynomial degree, especially in regions of strong field gradients or high particle density. This approach allows for increased numerical accuracy without a proportional increase in the number of mesh elements. By combining high-order basis functions with adaptive mesh refinement, the number of degrees of freedom can be significantly reduced while preserving the accuracy required for predictive beam dynamics simulations.

The presented methodology is demonstrated on a realistic negative ion beamline geometry, highlighting its efficiency and accuracy and showing its potential for future large-scale optimization studies of beam transport and guidance systems.

ACKNOWLEDGEMENTS

This work is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 516238647 – SFB 1667/1 (ATLAS - Advancing Technologies of Very Low-Altitude Satellites).

REFERENCES

[1] C.-D. Munz, M. Auweter-Kurtz, S. Fasoulas, A. Mirza, P. Ortwein, M. Pfeiffer, T. Stindl, “Coupled particle-in-cell and direct simulation Monte Carlo method for simulating reactive plasma flows,” (2014).

[2] S. Fasoulas, C.-D. Munz, M. Pfeiffer, J. Beyer, T. Binder, S. Copplestone, A. Mirza, P. Nizenkov, P. Ortwein, W. Reschke, “Combining particle-in-cell and direct simulation Monte Carlo for the simulation of reactive plasma flows,” (2019).

Kinetic Modeling of Argon DC Glow Discharge Using PIC/MCC and Comparison with Laser Absorption Measurements

Hsu Chang, He[1] and Sean O'Byrne[1,a)]

[1]*School of Engineering, College of Systems and Society, The Australian National University, Canberra, ACT 2601, Australia*

[a)]Corresponding author: sean.obyrne@anu.edu.au

Numerical modeling of DC glow discharges has been extensively studied over the past decades [1]. Argon is an ideal candidate for model validation as it is a noble gas and its properties can be precisely determined by *ab initio* calculations. Laser absorption spectroscopy enables quantitative measurements of argon metastable densities under discharge conditions, providing a reliable basis for comparison between experiments and simulations [2]. These capabilities make argon DC glow discharge an excellent benchmark case for validating kinetic plasma simulations.

Fig. 1 shows a diode-laser scan of an argon transition line. The laser temperature was held constant while the drive current was swept to cover the argon transition frequency. An autobalanced detector was used to record the log ratio signal, which was converted to absorbance, as shown in Fig. 1. Preliminary measurements were performed with pressure: 133.3 Pa and 1000 V discharge condition. The gas temperature and metastable argon number density were quantitatively determined assuming Doppler broadening and the Beer–Lambert law for absorption. The inferred metastable argon temperature was 1942 K, and the corresponding metastable number density was on the order of 10^7 cm^3. These measurements provide a quantitative basis for validation of the numerical model.

Previous numerical studies by Bogaerts and co-workers identified electron, ion, and fast neutral impact excitation as the dominant production mechanisms of excited argon states[3, 4]. Cascading from higher 4p levels was shown to be non-negligible under conditions where radiative processes are comparable to collisions [4]. Diffusion to the wall constitutes the primary loss mechanism, while electron quenching to resonant 4s states, pooling ionization, and Penning ionization may also become significant depending on discharge conditions. Accurate modeling of level-resolved argon excitation therefore requires a self-consistent kinetic description of charged particle transport and collision processes, motivating the use of a particle-in-cell/Monte Carlo collision (PIC/MCC) approach, which is well developed in late 1990[5].

In this work, a DC glow discharge with argon excited between two parallel plate electrodes is simulated using the Java-based PIC code Starfish. Charged particle dynamics under an applied electric field are resolved using PIC, with fast particles treated via MCC methods and slow species modeled as fluid equations. The numerical predictions of metastable argon densities will be compared with laser absorption spectroscopy measurements to assess the model's capability to accurately predict metastable populations under varying discharge conditions.

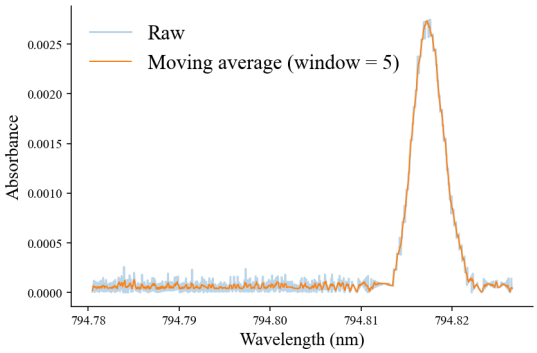


Fig. 1. Diode laser scanning of metastable argon transition line.

REFERENCES

[1] A. Bogaerts, R. Gijbels, *Vacuum* **69**, 37–52 (2002).
[2] T. Makabe, *Journal of Physics D: Applied Physics* **52**, 213002 (2019).
[3] A. Bogaerts, R. Gijbels, *Physical Review A* **52**, 3743 (1995).
[4] A. Bogaerts, R. Gijbels, J. Vlcek, *Journal of Applied Physics* **84**, 121–136 (1998).
[5] V. Vahedi, M. Surendra, *Computer Physics Communications* **87**, 179–198 (1995).

Numerical Simulation of Chemically Reacting Wakes of Hypersonic Spheres Using Kestrel CFD

B. S. Martin[1,a)], R. B. MacDermott[1], and J. J. Redmond[1]

[1]U.S. Air Force Institute of Technology, Wright-Patterson Air Force Base, Dayton, Ohio 45433, USA

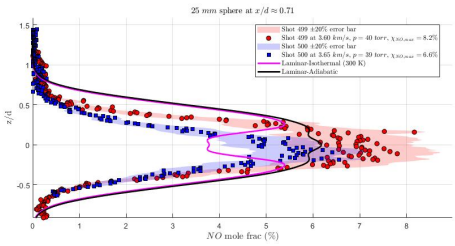
a)blake.martin.18.ctr@us.af.mil

Hypersonic wakes behind blunt bodies exhibit complex interactions between shock dynamics, rapid expansion, and thermochemical nonequilibrium. At Mach 10, finite-rate chemistry and vibrational nonequilibrium strongly influence wake species distributions, yet high-fidelity experimental datasets remain extremely limited. Conventional wind tunnel measurements are hindered by sting interference, and flight data rarely provide spatially resolved species information, placing hypersonic wakes in a transitional non-equilibrium regime where continuum and turbulence assumptions are challenged.

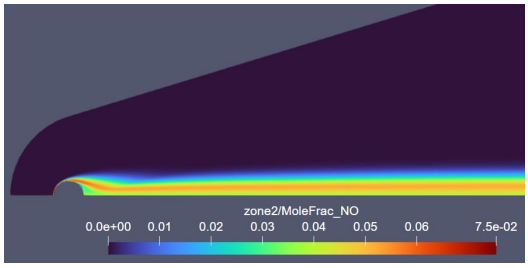
Recent ballistic free-flight experiments at Southwest Research Institute (SwRI) by MacDermott et al. [1] provide nitric oxide (NO) mole fraction measurements in the wake of 25 mm spheres at Mach 10 using high-repetition-rate planar laser-induced fluorescence (PLIF). Measurements extend up to 60 body diameters downstream and offer a rare opportunity to assess computational models of nonequilibrium hypersonic wakes.

Two-dimensional axisymmetric laminar simulations are performed using the Kestrel CFD [2] solver with the Park (1987) [3] two-temperature, five-species air model. Freestream conditions correspond to 3600 m/s, 5333 Pa, and 300 K. The sphere surface is modeled using both adiabatic and isothermal boundary conditions with a fully catalytic wall. The aluminum sphere has a very small Biot number ($\mathrm{Bi} \approx 0.004$), and combined with the extremely short test duration (200 μs), the sphere temperature can be assumed uniform.

For the laminar simulations, the adiabatic wall produces a χ_{NO} profile that rises more rapidly and reaches its peak further from the wake centerline compared to the experimental data. In contrast, the isothermal wall results in a χ_{NO} rise that aligns more closely with the measured peak location, but exhibits a pronounced drop along the wake centerline.



(a) Experimental and computational NO mole fraction profiles at $x/d = 0.71$.



(b) NO mole fraction contours from the laminar isothermal axisymmetric simulation.

Figure 1: Comparison of experimental PLIF measurements and Kestrel CFD predictions of NO mole fraction in the Mach 10 sphere wake.

Preliminary three-dimensional simulations have been conducted using mesh-adaptive off-body solvers for inviscid perfect-gas conditions. Expanding to fully three-dimensional, chemically reacting RANS simulations will eliminate numerical artifacts associated with axisymmetric formulations and enable direct comparison with experimental PLIF data.

Acknowledgements

The authors thank Southwest Research Institute for collaborating in collecting the Mach 10 sphere PLIF dataset.

This work was supported by the Air Force Institute of Technology using Department of the Air Force funds.

Distribution Unlimited; Approved for Public Release. AFRL Public Affairs Release Approval #AFRL-2026-0658. The views expressed are those of the author(s) and do not necessarily reflect the official policy or position of the Department of the Air Force, the Department of War, or the U.S. government.

References

[1] R. B. MacDermott, N. J. Meuschke, N. Jiang, P. S. Hsu, and S. Roy. *Applied Optics*, 64:D59–D56, 2025.

[2] CREATE-AV Department of Defense High Performance Computing Modernization Program (DoD HPCMP). Kestrel [version 11.1], 2023.

[3] C. Park. On the two-temperature model of chemically reacting flows. In *Proceedings of the 21st Thermophysics Conference*, number 87-1574 in AIAA Paper, 1987.

[4] J. D. Anderson. *Computational Fluid Dynamics*. McGraw Hill, 1st edition, 1995.

[5] L. Lees. Hypersonic wakes and trails. *AIAA Journal*, 2(3):417–428, 1964.

[6] Kitware, Inc. Paraview, 2023.

[7] C. Park. Assessment of a two-temperature kinetic model for ionizing air. *Journal of Thermophysics and Heat Transfer*, 3(3):233–244, 1989.

[8] C. Park. *Nonequilibrium Hypersonic Aerothermodynamics*. John Wiley & Sons, New York, NY, 1990.

[9] C. Park. Review of chemical-kinetic problems of future nasa missions, I: Earth entries. *Journal of Thermophysics and Heat Transfer*, 7(3):385–398, 1993.

Saturated Absorption Velocimetry in the Freestream of a High-Enthalpy Shock Tunnel Flow

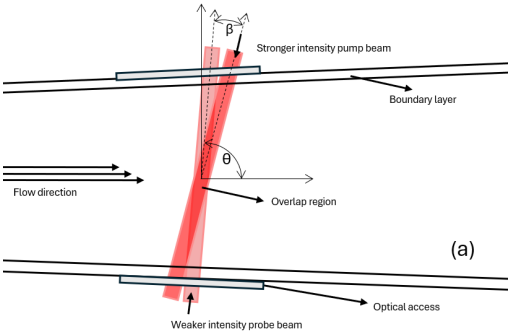
S. Roy[1,a)] and S. O'Byrne[1]

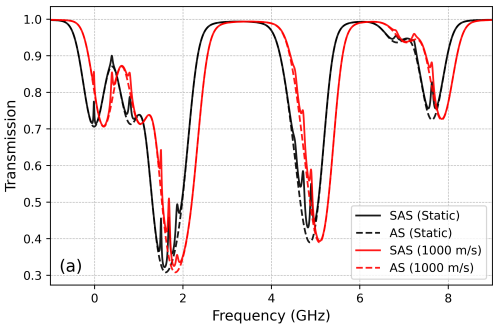
[1]*Australian National University, Australia*

[a)]Corresponding author: Swapneel.Roy@anu.edu.au

We present a Doppler-free laser absorption velocimetry technique for precise, spatially resolved velocity measurements in the freestream of the recently recommissioned T2 free-piston shock tunnel at the Australian National University. The method addresses the line-of-sight limitations of conventional tuneable diode laser absorption spectroscopy (TDLAS) by tracking changes in the sub-Doppler resonance contrast relative to the Doppler-shifted absorption background, enabling a local velocity measurement. The technique is non- intrusive, provides high signal-to-noise ratio with trace seeding, and enables both spatial and temporal resolution in low-density, high-Mach-number flows. The method requires seeding the shock-tunnel flow with rubidium chloride, which thermally dissociates to form atomic rubidium under the high-enthalpy conditions achieved within the test time [1]. A diode laser is split into counter-propagating pump and probe beams, generating narrow sub-Doppler resonances (Lamb dips) embedded within the Doppler-broadened absorption profile. These resonances have a spectral half-width of approximately ~6 MHz, compared with a Doppler width of approximately ~600 MHz [2] at room temperature. The Lamb dips act as zero-velocity markers within the atomic velocity distribution. When the beams intersect in the freestream, the Doppler-broadened profile shifts due to bulk flow velocity, while the intrinsic zero-velocity reference defined by the sub-Doppler resonance remains fixed in the laboratory frame as shown in figure (b) [2]. The resulting change in dip amplitude provides a direct measure of the local flow velocity within the beam overlap region (figure a). Because the signal originates only from this localized interaction volume, the technique mitigates the path- integration limitations inherent to conventional absorption-based velocimetry.

This paper presents experimental validation of previously developed modelling [2], demonstrating proof-of-concept operation in hypersonic flow. The sensitivity of the measurement to wavelength detuning, beam inclination angle and seed population is also quantified.





References

[1] Roy, S. and O'Byrne, S., 2024. Doppler-free saturated absorption velocimetry for low-density hypersonic flow diagnostics. In *AIP Conference Proceedings* (Vol. 2996, No. 1, p. 140004). AIP Publishing LLC.

[2] Roy, S., Thomas, R.J., Close, J.D. and O'Byrne, S., 2025. Saturated absorption spectroscopy for spatially resolved flow velocimetry. *Applied Optics*, 65(2), pp.390–399.

Electromagnetic flow control in hypersonic rarefied environment

Zhigang Pu[1] and **Kun Xu**[1,a)]

[1]*Department of Mathematics, Hong Kong University of Science and Technology, Hong Kong, China*

[a)]Corresponding author: makxu@ust.hk

The Unified Gas-Kinetic Wave-Particle (UGKWP) method, developed for the multiscale simulation of partially ionized plasmas, is applied to model electromagnetic flows around a hemisphere spanning regimes from near-continuum to rarefied conditions. To the best of our knowledge, this study presents the first application of a multiscale plasma solver to such a problem. In the formulation, neutrals, ions, and electrons are treated as distinct species. The numerical implementation is validated through comparisons with experimental data for a Mach 4.75 pre-ionized argon flow, where UGKWP results show close agreement with the experimental data. A further comparative study across different Knudsen numbers demonstrates that rarefaction effects weaken the influence of electromagnetic control. These findings highlight the capability of UGKWP in modeling electromagnetic control problems and underscore the significant role of rarefied effects in predicting flow-control behavior, thereby emphasizing the necessity of multiscale modeling in plasma flow applications [1, 2].

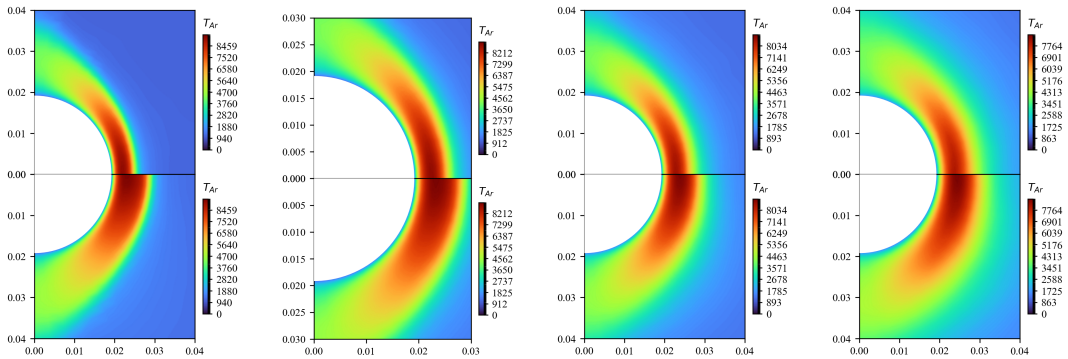


Fig. 1. Temperature contour plots of the argon atoms at (left to right) Kn=0.02, Kn=0.04, Kn=0.08, Kn=0.2 at $B_{max} = 0.447T$. Upper and lower figures refer to the results without and with external magnetic fields.

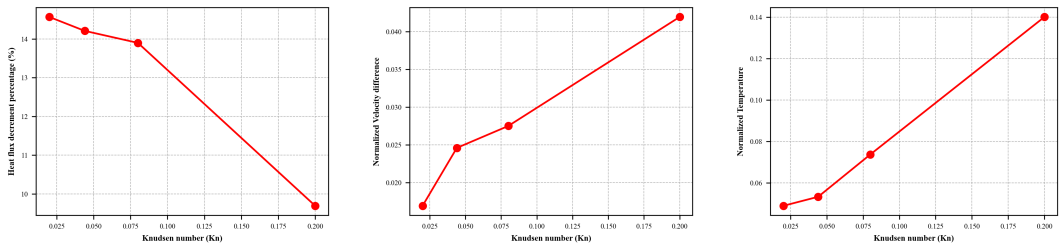


Fig. 2. (left) Heat flux decrement with varying Knudsen number. The maximum normalized velocity difference (middle) and maximum temperature difference (right) along the stagnation line between atoms and ions as functions of the Knudsen number

ACKNOWLEDGEMENTS

The first author would like to thank Wenpei Long, Junzhe Cao, Hongtao Liu and Shijie Qin for their valuable discussions on the project.

REFERENCES

[1] C. Liu, Y. Zhu, K. Xu, *Journal of Computational Physics* **401**, 108977 (2020).
[2] Z. Pu, K. Xu, *Journal of Computational Physics* **530**, 113918 (2025).

Modelling of plume–plume interactions in space like environment via the hybrid DSMC-Fokker–Planck approach

L. Basov[1,2,a] and M. Grabe[1]

[1]*Institute of Aerodynamics and Flow Technology, German Aerospace Center (DLR), Bunsenstrasse 10, Göttingen, 37073, Germany*
[2]*Applied and Computational Mathematics, RWTH Aachen, Schinkelstrasse 2, Aachen, 52062, Germany*

[a)]Corresponding author: leo.basov@dlr.de

Larger spacecraft typically use chemical propulsion systems for attitude and orbit control, or to maneuver during docking or landing. The thrusters operate by accelerating gas through a convergent-divergent nozzle, thus converting the gases internal energy to kinetic energy. In a vacuum environment, exhaust gases may interact with other vehicles or with the spacecraft itself, leading to undesired forces, heat fluxes, and potentially to a contamination of critical surfaces [1, 2]. Analysing plume expansion and interaction is therefore critical for spacecraft design.

Numerically studying thruster plumes in a high-vacuum environment is notoriously difficult, as the flow passes though a wide range of flow regimes, from high-density and low speed in the nozzle reservoir, to low-density, high-speed, non-equilibrium flow downstream of the nozzle exit.

The Direct Simulation Monte Carlo (DSMC) method [3] has been proven to be well suited to model rarefied and non-equilibrium flows. However, the method would be impractical in high-density regions of the plume, because of the computational cost incurred by computing inter-particle collisions. This problem has previously been tackled using hybrid continuum–particle methods. In this approach, the high-density region of the flow is treated with a Navier-Stokes solver, with the border of the continuum simulation domain providing the inflow conditions for the DSMC domain [4–6].

Whenever an expanding thruster plume interacts with adjacent surfaces, or the plume of a neighboring thruster, new areas of higher gas density form. These plume interaction zones produce flow patterns, that can have an appreciable impact on the surface pressure and heat flux [7]. To compute these areas of interaction with a hybrid approach, a spatially flexible, two-way coupling between code domains is required.

We propose to use a coupled particle-particle method, in which the low-density domains of the flow are simulated using DSMC, and the high density areas are modeled by an approximated Boltzmann equation. One such approximation to the Boltzmann equation is the Fokker–Planck (FP) equation, which can be solved using a particle approach particularly compatible with DSMC [8, 9]: particle transport, and the treatment of the boundary conditions, is identical to DSMC. Merely updating the post-collision properties of the simulator particles is handled differently, thus a hybrid method can be be implemented with relatively minor modification to an existing DSMC code. This approach was shown to be an efficient way to model two-way coupled flows [10] and has been applied to simulations of single plumes, as well as to their interaction with a surface [11].

In this paper, we present results of a two-way coupled, hybrid DSMC-FP simulation of plume-plume interaction in a dual thurster configuration to demonstrate the feasibility of the approach for large scale applications.

REFERENCES

[1] G. Dettleff, *Progress in Aerospace Sciences* **28**, 1–71January (1991).
[2] G. Dettleff, M. Grabe, "Basics of Plume Impingement Analysis for Small Chemical and Cold Gas Thrusters," NATO Report RTO-EN-AVT-194 (DLR, Göttingen, 2011).
[3] G. A. Bird, *Molecular Gas Dynamics and the direct Simulation of Gas Flows* (Oxford University Press, New York, 1994).
[4] D. Hash, H. Hassan, "A hybrid DSMC/Navier-Stokes solver," in *33rd Aerospace Sciences Meeting and Exhibit*.
[5] T. Schwartzentruber, L. Scalabrin, I. Boyd, "Modular implementation of a hybrid DSMC-NS algorithm for hypersonic non-equilibrium flows," in *45th AIAA Aerospace Sciences Meeting and Exhibit*.
[6] C. Virgile, A. Albert, L. Julien, **195**, 295–308.
[7] H. Tani, T. Ohmaru, *Journal of Spacecraft and Rockets* **59**, 660–673March (2022).
[8] P. Jenny, M. Torrilhon, S. Heinz, *Journal of Computational Physics* **229**, 1077–1098February (2010).
[9] M. H. Gorji, M. Torrilhon, P. Jenny, *Journal of Fluid Mechanics* **680**, 574–601August (2011).
[10] M. H. Gorji, P. Jenny, *Journal of Computational Physics* **287**, 110–129April (2015).
[11] C. Hepp, "A kinetic Fokker-Planck algorithm for simulating multiscale gas flows," Dissertation, JLU Giessen, Giessen 2022.

Abstract 148

Comprehensive cross section datasets for charged particle collisions with atoms and molecules

D. V. Fursa[1,a)], L. H. Scarlett[1], H. Umer[1], C. T. Plowman[1], I. Bray[1], M. C. Zammit[2], M. V. Pak[3], R. C. Bergmayr[4], D. Wunderlich[4], and U. Fantz[4]

[1]*Department of Physics and Astronomy, Curtin University, Perth, Western Australia 6102, Australia*
[2]*Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[3]*Department of Physics, Air Force Institute of Technology, Wright-Patterson AFB, Ohio 45433, USA*
[4]*Max Planck Institute for Plasma Physics, Boltzmannstraße 2, Garching, 85748, Germany*

[a)] Corresponding author: d.fursa@curtin.edu.au

Charged particle (electrons, positrons, ions) collisions with atoms, ions, and molecules play an important role in understanding the properties and dynamics of various plasmas originating from industrial applications, as well as astrophysical, atmospheric, and fusion research. Plasma modelling tools, such as particle-in-cell codes with Monte Carlo methods for collisions, Boltzmann equation solvers, and fluid models, rely on fundamental input data (scattering cross sections) to simulate the collective dynamics of charged particles and gain an understanding of macroscopic plasma properties. The accuracy of the input cross sections will obviously determine the accuracy of the simulation results. Historically, accurate collision experiments have been the main source of cross section datasets used in plasma modelling. However, the experimental data are often sparse and available for a few collision systems. The remarkable progress in computer power and the development of modern computational infrastructure over the last few decades have made computational techniques the primary supplier of accurate and comprehensive collision data. I will highlight the recent developments in the field of computational collision physics and illustrate them using the examples drawn from the development and applications of the Convergent Close-Coupling method [1,2,3] to modelling collision processes. Comprehensive sets of collision cross sections are currently available for several collision systems, for example, for electron collisions with hydrogen [4] and helium atoms [5] and hydrogen molecules [6]. The utility of the molecular hydrogen collision data set (hundreds of thousands of entries for electron projectile [7]) in establishing detailed collision radiative models for low-temperature hydrogen plasmas [8] will be discussed.

ACKNOWLEDGEMENTS

This work was supported by the Australian Research Council, the Pawsey Supercomputing Centre, the European Union via the Euratom Research and Training Programme, Los Alamos National Laboratory, and the U. S. Air Force Office of Scientific Research.

REFERENCES

[1] I. Bray *et al.*, *J. Phys. B: At. Mol. Opt. Phys,* **35**, p. R117 (2002).
[2] M. C. Zammit *et al.*, *J. Phys. B: At. Mol. Opt. Phys*. **50**, p. 123001(2017).
[3] C. T. Plowman *et al.*, *Phys. Rev. A*, **112**, 042811 (2025).
[4] I. Bray and A. T. Stelbovics, *Phys. Rev. A,* **46**, 6995 (1992)
[5] Yu. Ralchenko *et al.*, *At. Data Nucl. Data Tables,* **94**, p. 603 (2008).
[6] L. H. Scarlett *et al.*, *At. Data Nucl. Data Tables,* **137**, p.101361 (2021).
[7] MCCC database: mccc-db.org
[8] R. C. Bergmayr *et al.*, *J. Quant. Spectrosc. Radiat. Transfer*, **338**, p. 109414 (2025)

Design of a Test Model for Studying Gas Surface Interactions in Ablating Flows

Henry G. B. Straede[1,a)], Samuel G. Lock[1], Timothy J. McIntyre[1], Richard G. Morgan[1] and Christopher M. James[1]

[1]*The University of Queensland, St Lucia, QLD, 4072, Australia*

[a)]Corresponding author: h.straede@uq.edu.au

Gas surface reactions on ablative heat transfer materials in hypersonic flows has long been a difficult problem to solve. A major reason for this is the lack of experimental data that simulate the real environments seen by vehicles. A large amount of data is available for molecular beam experiments which help to understand the ablation phenomena without the need for a flow. Arc-jet facilities are also commonly used as a way to generate experimental ablation data due to the long test times. The flows in these facilities are however, not fully representative of real hypersonic flight due to the low enthalpy generated.

UQ's X2 expansion tube is a free-piston driven facility that is capable of replicating the enthalpy of high-speed flight over a scaled model. The limitation of this is the shortened test times meaning that the model is required to be pre-heated. In 2013, Fabian Zander developed a technique to perform experiments with resistively heated test models in UQ's X2 Expansion Tube [1]. This can be used to pre-heat carbon based samples to the required temperature to induce ablation within the short test times of the facility.

Furthermore, the majority of past experiments have focused exclusively on the measurement of the ablation product CN, due to its relative abundance. UQ's upgraded emission spectroscopy system is capable of measuring a larger array of wavelengths during the same experiment. This will enable the measurement of more radiating species than previously possible.

Recent projects that have employed the heated model technique in X2 are Steven Lewis in 2017 [2] to Nils Temme [3] and Ranjith Ravinchandran [4] in 2022. These experiments show large variation in the chosen test model geometry, material and heating temperature to suit the specific aims of each study.

This paper and the associated presentation will outline preliminary test model designs and simulations for an upcoming study of ablation products in the wake of hypersonic vehicles. This can generate a greater understanding of the reactions and reaction rates present on the surface of ablative materials. These experiments will be informed by and results compared to computational modeling of the gas surface interactions to be performed by the United States Air Force Institute of Technology (AFIT).

The experiments will target the wake of the model, thus it is important to understand whether the geometry is capable of developing a wake or near-wake within the test times of X2. The geometry must also ensure that there is sufficient interaction between the flow and the heated element to allow reactions to occur and be seen downstream. These requirements will be investigated using preliminary CFD modeling.

Another important consideration is the ability of the model to be resistively heated to a sufficient temperature. This is a complex problem that is dependent on the chosen material and its geometry. Analytical calculations along with finite element analysis of the different test model options will be presented to address this consideration.

This presentation will focus on the heated portion of the model and the geometry relevant for the flow structure. It will not contain a full model design with the model mount, electrical connections, isolators and insulators.

ACKNOWLEDGEMENTS

This work is supported by the Air Force Office of Scientific Research under award number FA2386-25-1-4032. Henry Straede is the recipient of an Australian government Research Training Program scholarship.

REFERENCES

[1] F. Zander, R. G. Morgan, U. Sheikh, D. R. Buttsworth, P. R. Teakle, *AIAA Journal* **51**, 476–484 (2013), https://doi.org/10.2514/1.J051867 .

[2] S. W. Lewis, C. M. James, R. G. Morgan, T. J. McIntyre, C. R. Alba, R. B. Greendyke, *Journal of thermophysics and heat transfer* **31**, 193–204 (2017).

[3] N. Temme, *Hypervelocity boundary-layer flow experiments with high surface temperature ablation* (The University of Queensland, School of Mechanical and Mining Engineering, 2022).

[4] R. Ravichandran, S. W. Lewis, C. M. James, R. G. Morgan, T. J. McIntyre, *Journal of thermophysics and heat transfer* **35**, 335–348 (2021).

[5] *Design and Testing of a Heated, Ablating Blunted Wedge Model*.

Vibrational Non-Boltzmann Effects in Advection-dominated Boundary Layer Flows

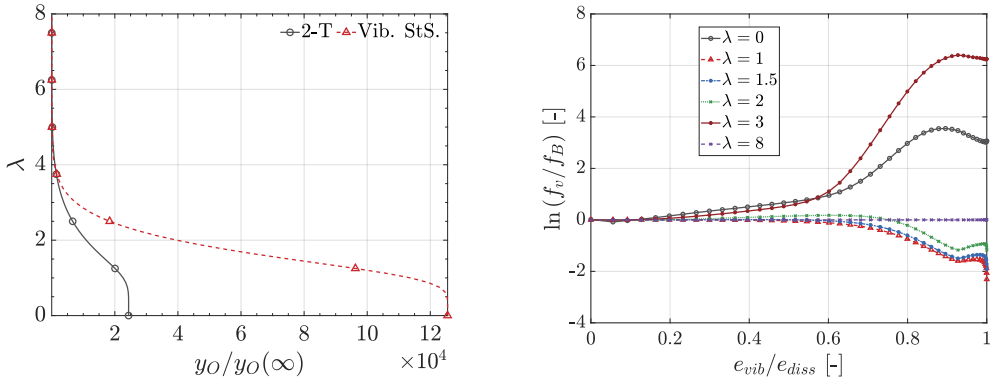
S. Ravichandran[1] and R. L. Macdonald[1,a)]

[1]*Ann and H. J. Smead Aerospace Engineering Sciences, University of Colorado Boulder, USA.*

[a)]Corresponding author: robyn.macdonald@colorado.edu
Oral Presentation

Advection-dominated hypersonic boundary layers are typically formed over slender geometries, such as blunt-nosed wedges or cones. These boundary layers are characterized by cold walls, which cause a sharp temperature drop from a peak value. The most commonly used approach to model vibrational nonequilibrium is the two-temperature (2-T) model which relies on the assumption of equilibrium among vibrational energy states at a mode temperature. However, vibrational non-Boltzmann distributions may arise in the near-wall region due to temperature gradients. These, in turn, may affect radiative heating and transition to turbulence on vehicle surfaces.

This work employs a computationally inexpensive locally self-similar formulation [1] to analyze steady laminar boundary layers with vibrational state-to-state (Vib. StS) thermochemistry. Fig. 1a. shows differences between normalized atomic oxygen concentrations predicted using 2-T and vibrational StS models for a non-catalytic wall. While both models predict net dissociation of oxygen due to the temperature peak, vibrational StS predicts a greater increase in oxygen atom mass fraction than 2-T. Fig. 1b. shows a measure of deviation from Boltzmann distributions within the boundary layer. Non-Boltzmann populations of higher vibrational states occur close to the wall ($\lambda \leq 3$) possibly due to temperature gradients. At the wall ($\lambda = 0$) the vibrational state distribution shows a significant deviation from a Boltzmann distribution with high vibrational states being overpopulated.



(a) **(b)**

Fig. 1. (a) Normalized O-atom mass fractions, and (b) Logarithm of local-to-Boltzmann populations of O_2, within boundary layer with freestream velocity 6,000 m/s, wall-to-freestream temperature ratio 1.33, and non-catalytic wall, at a streamwise location of 50 mm.

The final paper will aim to understand the complex interplay between vibrational and chemical nonequilibrium within laminar boundary layers, and their contributions to wall heating and skin friction. Vibrational StS databases obtained from Forced Harmonic Oscillator and Quasiclassical Trajectories [2, 3] will be used for comparison.

ACKNOWLEDGEMENTS

We acknowledge funding support from Air Force Office of Scientific Research under the Young Investigator Program, Grant No. FA9550-22-1-0188, with Program Officer Dr. Amanda Chou.

REFERENCES

[1] A. Liñán Martínez, I. Da Riva de la Cavada, ICAS : Third Congress, Stockholm (Spartan Books, Washington, 1964).
[2] M. Lino da Silva, J. Loureiro, V. Guerra, Chemical Physics Letters **531**, 28–33 (2012).
[3] V. T. Baluckram, D. Andrienko, AIAA Scitech 2020 Forum (2020).

Abstract 152

From sparse diagnostics to plume fields: what can (not) be inferred with PINN–PONN reconstruction?

Nadim Maraqten[1,a)], Georg Herdrich[1] and Uwe Soergel[2]

[1]*Institute of Space Systems, University of Stuttgart, Stuttgart, 70569, Germany*
[2]*Institute for Photogrammetry and Geoinformatics, University of Stuttgart, Stuttgart, 70569, Germany*

[a)]Corresponding author: nadim.maraqten@irs.uni-stuttgart.de

Although numerical simulations can characterize plasma plume expansion in considerable detail within specific regimes, obtaining a single consistent description across collisional, transitional, and rarefied conditions often requires changing both the physical model and the numerical approach (e.g., continuum-fluid, kinetic, or hybrid treatments). Experimental characterization is likewise fundamentally constrained by measurement sparsity: dense probe scans can be invasive and resource-intensive, whereas non-intrusive Laser-Induced Fluorescence (LIF) is often limited to sparse spatial sampling due to acquisition overhead. Motivated by these complementary limitations, we investigate how much plume-field information can be inferred from sparse velocity data using the Physics-Informed Neural Network Plasma flOw recoNstructioN (PINN–PONN) framework [1], a physics-informed data-assimilation approach that reconstructs 2-D macroscopic plume fields by combining (a) local measurements, (b) global facility observables, and regularizing with (c) convective conservation terms (Fig. 1).

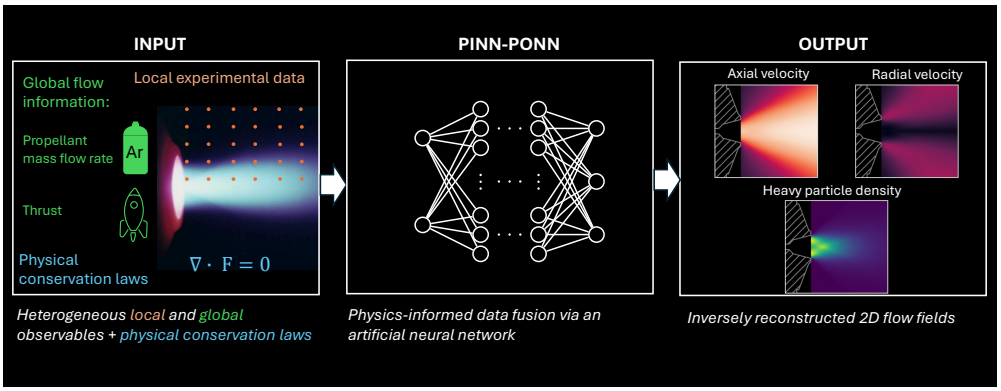


Fig. 1. Overview of the PINN–PONN data-fusion and reconstruction workflow.

We quantify resolution–error scaling by subsampling synthetic LIF-like velocity measurements from an experimentally validated magnetoplasmadynamic thruster plume simulation, providing a controlled reference for assessing reconstruction error. We vary the measurement-grid resolution while keeping the sampling geometry fixed, and regularize the ill-posed inverse problem using mass-flow rate, thrust, and convective mass/momentum/energy conservation-law residuals. We test for a diminishing-returns regime in velocity-field error versus measurement-grid resolution, with a knee beyond which additional samples yield limited improvements. We estimate uncertainty due to inverse ill-posedness (epistemic) via multi-start ensemble reconstructions and assess empirical coverage against the simulation reference. We further examine when heavy-particle density is (not) identifiable from velocity-only inputs and report residual non-uniqueness as ensemble-based uncertainty in the inferred density field.

These results provide an effort-aware sampling roadmap for sparse optical diagnostics and delineate when physics-informed reconstruction can (and cannot) recover macroscopic 2-D plume structure from sparse velocity measurements.

REFERENCES

[1] N. Maraqten, O. Nimer, J. Grill, M. Ehresmann, U. Soergel, G. Herdrich, "PINN–PONN: A Novel Physics-Informed Deep Learning Method for Plasma Flow Reconstruction," *Proceedings of the 39th International Electric Propulsion Conference (IEPC-2025)* (London, United Kingdom, 2025) Paper IEPC-2025-287.

Abstract 154

Modelling Characteristic Disturbances in Impulse Facilities

Noah Wechgelaer[1,a)], Toby J. van den Herik[1] and Christopher M. James[1]

[1] *The University of Queensland, St Lucia, QLD, 4072, Australia*

[a)] Corresponding author: n.wechgelaer@gmail.com

Impulse facilities—such as shock tubes, expansion tubes, and reflected shock tunnels—are critical experimental platforms for studying high-enthalpy, high-speed flows relevant to hypersonics, atmospheric entry, and propulsion. Unlike continuous-flow wind tunnels, impulse facilities generate short-duration test flows (typically microseconds to milliseconds) by rapidly releasing stored energy. While these facilities enable access to extreme thermodynamic conditions, the transient nature of their operation introduces characteristic disturbances that can significantly affect flow quality, test time, and data interpretation. Accurate modelling of these disturbances is therefore essential for reliable experiment design, facility optimisation, and uncertainty quantification.

The modelling of these characteristic disturbances was performed by utilising L1d [1], a CFD (Computational-Fluid-Dynamics) code, and the resulting data was then manipulated to estimate these disturbances. An analysis of control conditions was done to observe any trends that different characteristic disturbances may cause. This was done by looking at cold driver conditions with no area change to reduce complexity, and manipulating initial conditions, such as shock tube fill pressures and driver length, to find the different terminating conditions. By observing the pitot pressure traces, different behaviours for different termination conditions were found. These could be used to analyse experimental data and predict the terminating condition that is cutting the test time short.

The three terminating conditions that were analysed were expansion front termination, reflected u+a termination, and driver disturbance termination. These three terminating conditions are important to understand when designing experiments, as through an understanding of these conditions, predicting, maximising test time and reducing disturbances can become easier.

Finally, to validate the characteristic disturbance model, a comparison between previously conducted experiments and L1d recreations of the experiments was done. This provides insight into the accuracy of the model and a better understanding of terminating disturbances.

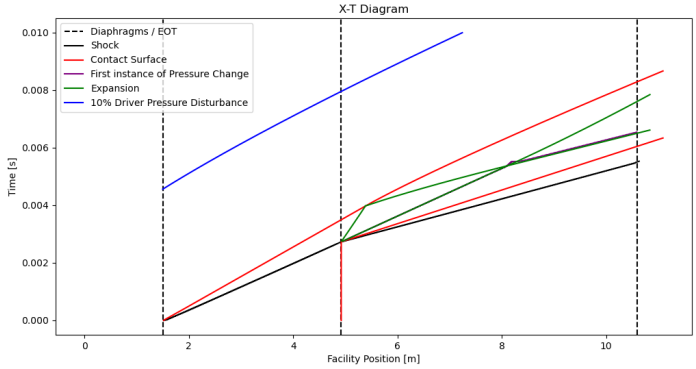


Fig. 1. Example of an x-t diagram, which graphs terminating conditions.

REFERENCES

[1] Jacobs, P. A. (1994). *Quasi-One-Dimensional Modeling of a Free-Piston Shock Tunnel.* University of Queensland, St. Lucia, Queensland 4072, Australia: AIAA JOURNAL.

Hypersonic Ground Testing Stagnation Point Thermography Using Foil Calorimeter

C. Yu[1,a)], D. E. Gildfind,[1], D. J. Mee,[1] and T. J. McIntyre[2]

[1]*The University of Queensland, School of Mechanical and Mining Engineering*
[2]*The University of Queensland, School of Mathematics and Physics*

[a)]Corresponding author: uqyche53@uq.edu.au

When a spacecraft re-enters Earth's atmosphere it is usually travelling at high hypervelocity speeds, and a strong bow shock forms over the blunt body. Kinetic energy is transferred to heat energy as the flow slows relative to the vehicle, with the temperature in the shock layer reaching orders of 15,000K [1]. This promotes the dissociation and ionisation of gas molecules in the shock layer, thereby liberating electrons and promoting plasma formation at the forebody of the capsule. Magnetohydrodynamic (MHD) aerobraking proposes equipping the spacecraft with a magnetic field generator, which is capable of interacting with the charged particles present in the high temperature shock layer due to Lorentz force. MHD is expected to significantly reduce total and peak heat transfer and beneficially enhance drag on the spacecraft, but compelling experimental data to confirm this expectation remains elusive [2].

Recent attempts to measure the effect of MHD flow control on heat flux in an expansion tube facility, with the models instrumented with thin film heat transfer gauges (TFHTGs) and thermocouples, demonstrated increased noise due to the highly ionised shock layer and the presence of a magnetic field. The uncertainties in the measurement of total heat flux at the stagnation point increased from 8.0% to 16.2%, and in some cases could not be measured due to overwhelming electrical noise [3]. This highlights the need for optical heat flux measurement methodologies that are more electromagnetic-interference (EMI) resistant. Conventional thermography is limited by the hot and radiative shock layer in the optical path, which can obscure radiation emitted by the model surface. The proof of concept for an optical, through-model, metal foil calorimeter method, where the shock layer is eliminated, was demonstrated in earlier experiments on a flat plate. The full paper aims to adapt this methodology to a blunt body model where the calorimeter is expected to measure stagnation point heat flux.

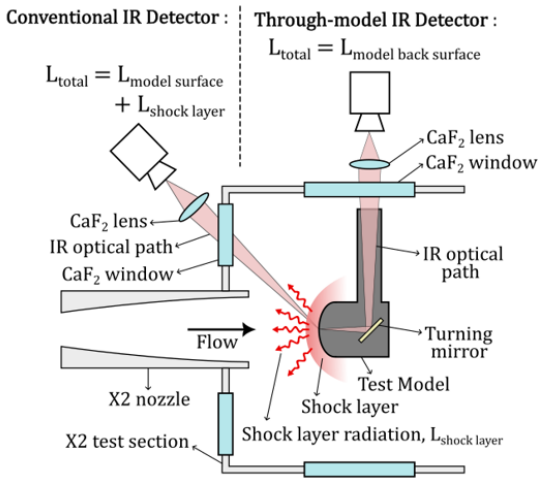


Fig. 1. Labelled schematic of through-model thermography for blunt body as compared to conventional thermography

ACKNOWLEDGEMENTS

C. Yu is a recipient of the Research Training Scholarship of UQ. This research was supported by the Australian Government through the Australian Research Council's Discovery Projects funding scheme (DP220101478).

REFERENCES

[1] J. D. Anderson Jr., *Hypersonic and High-Temperature Gas Dynamics, Second Edition* (American Institute of Aeronautics and Astronautics, 2006-10-31).
[2] R. C. Meyer, *Journal of the Aerospace Sciences* **25**, 561–566 (1958-09).
[3] A. Lefevre, D. E. Gildfind, R. J. Gollan, P. A. Jacobs, C. M. James, *AIAA Journal* **60**, 5046–5059 (2022-09).

Self-thermophoresis of a Thin Circular Disk

T. Tomita[1], S. Taguchi[1,a)] and T. Tsuji[1]

[1]*Department of Informatics, Graduate School of Informatics, Kyoto University, Kyoto 606-8501, Japan*

[a)]Corresponding author: taguchi.satoshi.5a@kyoto-u.ac.jp

In a rarefied gas, a body with a non-uniform temperature distribution induces a flow around the body and receives a recoil force from the gas, resulting in a self-induced motion (self-thermophoresis). A classical example is a vane of the Crookes radiometer, which has a temperature difference between both sides. The gas molecules reflected on the hotter side deprive the vane of greater momentum on average, yielding a total net momentum exchange between the vane and the gas. The resulting force, particularly referred to as the radiometric force, drives the vane from the hotter to colder side. Since the temperature difference can be established by light absorption, this mechanism can also be regarded as a source of a photophoretic force, and its application to aerosol engineering and near-space flight has been considered and implemented (e.g., [1]). According to the kinetic theory of gases, the spatially steep variations of the macroscopic quantities near the sharp edge of a thin body are closely connected to the discontinuities of the velocity distribution function (VDF), arising at the edge and propagating into the gas region [2]. In this study, we numerically investigate thermally-induced flows around an infinitely thin circular disk with one side heated and calculate the radiometric forces, with a particular emphasis on the precise treatment of the discontinuities of the VDF. While a spatially three-dimensional problem was numerically analyzed in [3], the above-mentioned special role of the sharp edge has not been tackled in the literature. Furthermore, in order to eliminate the effect of external walls, we consider the infinite expanse of the gas. By solidly dealing with such delicate problems concealed in the simple configuration, we aim to develop the reference numerical data of the radiometric force and the settling velocity with high precision.

The problem considered in the study is as follows. An infinitely thin circular disk with radius L freely moves in a rarefied gas (Fig. 1). Far from the disk, the gas is in the equilibrium state at rest with the density ρ_0 and the temperature T_0. One side of the disk is slightly heated and kept at a uniform temperature $T_0(1+\tau_\mathrm{w})$ ($\tau_\mathrm{w} > 0$), while the other side is kept at the uniform temperature same as at infinity, say, T_0. The disk receives a radiometric force in a perpendicular direction to itself and undergoes translational motion. The terminal velocity of the disk, denoted by U_*, is achieved when the radiometric and drag forces counterbalance each other. Provided that the velocity of the disk has settled, we investigate the radiometric force, the terminal velocity of the disk, and the behavior of the gas around the disk on the basis of the Bhatnagar–Gross–Krook model of the Boltzmann equation and the diffuse reflection boundary condition. Here, we suppose that the temperature perturbation τ_w and the normalized terminal velocity $u_* = U_*(2RT_0)^{-1/2}$ are so small (i.e., $\tau_\mathrm{w} \ll 1$, $u_* \ll 1$) that the system can be linearized around the reference equilibrium state at rest with the density ρ_0 and the temperature T_0, where R is the specific gas constant. The (global) Knudsen number Kn is defined by the ratio of the mean free path in the reference equilibrium state at rest, ℓ_0, to the disk radius L, that is, $\mathrm{Kn} = \ell_0/L$.

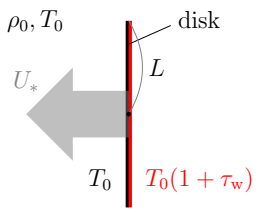


FIGURE 1. Problem.

By taking a frame moving with the disk, the uniform linear motion of the disk with speed U_* is transformed into the uniform flow past the disk with the same speed and the opposite direction, reducing to the steady boundary-value problem. However, U_* (or u_*) is determined as a response to the temperature perturbation τ_w, and thus we do not know its value beforehand. To resolve this issue, we draw on the approach used in [4]: Consider a slightly modified problem, where the speed of the uniform flow U is given as a control parameter. If we adjust U so that the drag force counterbalances the radiometric force, it just gives the terminal velocity in the original problem. We further exploit the linearity of the problem to decompose it into the auxiliary problems, not only making the adjustment of U semi-analytical, but also substantially reducing the physical parameters of concern. The auxiliary problems are numerically solved by the scheme based on the method of characteristics, constructed in [5]. The key advantage of this scheme is that the discontinuities of the VDF are properly preserved in the numerical solutions. In the talk, we will show our results for a wide range of Kn, including the comparison with some experimental and numerical data in the literature.

ACKNOWLEDGEMENTS

This work was supported by JSPS KAKENHI Grant Numbers JP22K03924, JP22K18770, JP25K01156 and JST SPRING Grant Number JPMJSP2110. Numerical computations were carried out using the supercomputer of ACCMS, Kyoto University.

REFERENCES

[1] B. C. Schafer, J.-H. Kim, F. Sharipov, G.-S. Hwang, J. J. Vlassak, D. W. Keith, *Nature* **644**, 362–369 (2025).
[2] S. Taguchi, K. Aoki, *Journal of Fluid Mechanics* **694**, 191–224 (2012).
[3] G. Dechristé, L. Mieussens, *Journal of Computational Physics* **314**, 465–488 (2016).
[4] S. Taguchi, K. Aoki, *Physical Review E* **91**, 063007 (2015).
[5] T. Tomita, S. Taguchi, T. Tsuji, *Journal of Fluid Mechanics* **1027**, A36 (2026).

Molecular Dynamics Study of Poiseuille Flow of Dense Confined Fluids

R. Kiyose[1], S. Taguchi,[1,a)] and T. Tsuji[1]

[1]*Department of Informatics, Graduate School of Informatics, Kyoto University, Kyoto 606-8501, Japan*

[a)]Corresponding author: taguchi.satoshi.5a@kyoto-u.ac.jp

In nanoscale systems, such as porous media with small pores and nano devices, the diameter of gas molecules can be comparable to the characteristic length or the mean free path of molecules. Although the Boltzmann equation is widely used for describing the behavior of the rarefied gas, its applicability is limited to an ideal-gas regime (the Boltzmann–Grad limit), in which molecular diameter is negligibly small to both the characteristic length and the mean free path. When molecular diameter is comparable to either of these two length scales mentioned above, the finite size of molecules needs be taken into account. There exist two main approaches to investigate the fluid behavior in this regime: the Enskog equation and its extensions within the framework of kinetic theory, and the other is molecular dynamics (MD) within the framework of Newtonian dynamics. The former describes velocity distribution function and yields transport coefficients in the continuum limit, but its collision term involves an approximation of molecular correlations. The latter computes molecular motion on the basis of microscopic dynamics, although it can be computationally demanding, especially when signal-to-noise ratio is low and a large number of samples is needed. In the present work, we employ molecular dynamics, given the recent advances in computational capabilities and the fact that MD captures molecular correlations without approximation.

To investigate finite molecular size effects, we study the behavior of gas composed of N molecules using molecular dynamics for Poiseuille flow between two parallel plates, which is known as a classical problem (Fig. 1). Gas molecules are modeled as identical hard spheres, and their interactions are assumed to be elastic. The plates are modeled as flat surfaces, and the gas-surface interactions are also modeled as diffuse reflection, which is widely applied in the rarefied gas dynamics, and the temperature of the plates is kept at constant and uniform. Considering the nature of our problem setting, in which molecular velocity changes instantaneously upon collision, we employed the event-driven molecular dynamics for precise and efficient computation [1, 2]. In this method, the state of the system jumps from the current time to the earliest collision event calculated in advance, and is then updated to the state after collision.

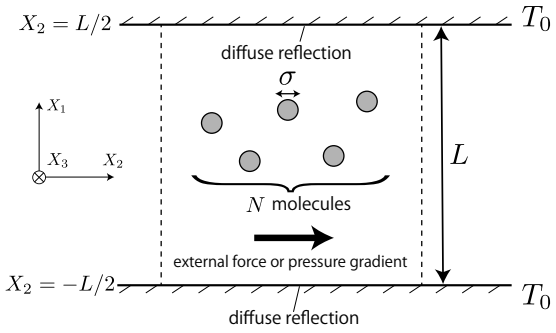


FIGURE 1. Schematic of the problem

Macroscopic quantities, such as mass flow rate, density, flow velocity, temperature are obtained from our MD, and we examine the relationship between macroscopic quantities and molecular diameter for various Knudsen numbers. To account for the transport of momentum and energy not only through molecular advection but also through intermolecular collision, macroscopic quantities such as stress and heat flow are computed using the method of planes [3]. Both force-driven and pressure-driven Poiseuille flow are investigated. According to the Boltzmann equation, the two flows are equivalent, whereas the Enskog equation suggests that they are not strictly equivalent, although the discrepancy remain small [4]. Profiles of density and stress at the reference state and mass flow rates obtained by our molecular dynamics show good agreement with those of the previous study based on the Enskog equation.

ACKNOWLEDGEMENTS

This work was supported by JSPS KAKENHI Grant Numbers JP25K01156 and JST SPRING Grant Number JPMJSP2110.

REFERENCES

[1] T. Pöschel, T. Schwager, *Computational Granular Dynamics* (Springer-Verlag, 2005), 13–134.
[2] S. Miller, S. Luding, *Journal of Computational Physics* **193**, 306–316 (2004).
[3] H. Kusudo, T. Omori, Y. Yamaguchi, *The Journal of Chemical Physics* **155** (2021).
[4] M. Hattori, *Journal of Fluid Mechanics* **962**, A20 (2023).

Numerical Study of Magnetohydrodynamic Aerobraking for Large-scale Spacecraft with Magnetic Field Deformation

S. B. van Oeveren[1,a)], D. E. Gildfind,[1], V. Wheatley[1] and R. J. Gollan[1]

[1] *University of Queensland, St. Lucia, Queensland, 4072, Australia*

[a)] s.vanoeveren@uq.net.au

High-velocity atmospheric entry subjects spacecraft to extreme aerodynamic and thermal loads. During entry, atmospheric gas is compressed in a shock layer ahead of the spacecraft, generating high temperatures that may produce an ionised plasma. Many thermal protection technologies, including magnetohydrodynamic (MHD) aerobraking, are investigated in the literature to manage the risks posed by these extreme conditions. MHD aerobraking involves generating a magnetic field from within the spacecraft that interacts with surrounding ionised plasma to produce Lorentz forces. These Lorentz forces can be leveraged to augment the shock layer, potentially enhancing drag and reducing convective heat loads. This phenomenon has been widely investigated in the literature. For example, experimental work by Lefevre et al. [1] demonstrated increased shock standoff for a spherical permanent magnet in a 13.8 km/s air flow, while computational studies by Shimosawa and Fujino [2] predicted enhanced drag and reduced convective heat flux for a magnetised sphere in a 12.4 km/s flow. However, such studies have focused primarily on relatively small, idealised spherical bodies. Applying MHD aerobraking to more practical entry scenarios, such as crewed spacecraft returning from the Moon, will require analysing larger and more complex spacecraft geometries. Such configurations introduce new challenges, including magnetic field deformation, which can alter the expected MHD performance.

The magnetic Reynolds number describes the tendency of a magnetic field to deform in a conductive fluid,

$$Re_m = \mu_0 \sigma u L, \tag{1}$$

where μ_0 is the vacuum permeability constant, σ is the flow conductivity, u is the velocity, and L is the characteristic length scale. For $Re_m < 1$ the magnetic field is generally assumed to remain relatively undeformed, however when $Re_m > 1$, advection of the magnetic field becomes more significant and the field may experience deformation. Large, high-velocity spacecraft are expected to generate $Re_m > 1$, suggesting that magnetic field deformation may significantly influence the MHD behaviour. This study will consider the lunar return of a theoretical MHD-assisted Orion capsule geometry, which is a 5 m diameter NASA crew module designed to return to Earth at velocities around 11 km/s. The aim is to assess the impact of magnetic field deformation on MHD flow control at high-velocity, large-scale flight conditions where $Re_m > 1$. Under these conditions the behaviour of the magnetic field must be solved using the resistive MHD formulation which couples the magnetic field behaviour into the Navier-Stokes equations to account for changes in the magnetic field. Fig. 1 presents preliminary simulations of a 0.8 m diameter, 0.2 T spherical magnet entering Earth at 11.8 km/s. The upper half of the figure corresponds to a solution that accounts for magnetic field deformation, while the lower half shows a solution that assumes a fixed, undeformed field. This comparison highlights the significant influence field deformation can have on MHD aerobraking. It can be seen that when field deformation is included, the predicted magnetic field and pressure distribution differ substantially from the fixed-field assumption, resulting in a 41% reduction in shock standoff distance, as shown in Fig. 1(b). The full paper will extend this analysis to a NASA Orion geometry to evaluate these large-scale, high-velocity effects on the MHD aerobraking concept.

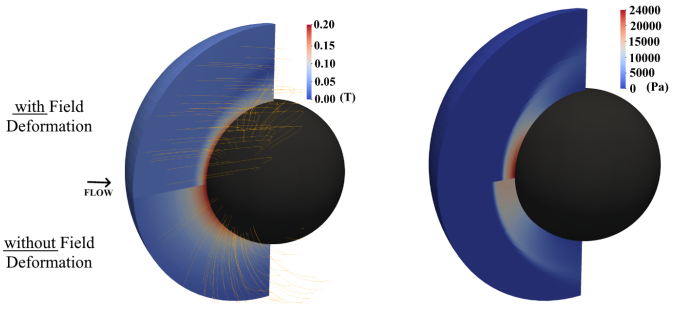


Fig. 1. Comparison of MHD solutions with a non-deformed magnetic field (lower half) and a deformed field (upper half) for a 0.8 m, 0.2 T spherical magnet at an 11.8 km/s entry condition.

REFERENCES

[1] A. Lefevre, D. E. Gildfind, R. J. Gollan, P. A. Jacobs, T. J. McIntyre, *AIAA Journal* **59**, 3228–3240 (2021).
[2] Y. Shimosawa, T. Fujino, *Journal of Spacecraft and Rockets* **53**, 528–537 (2016).

Vacuum Ultraviolet to Near-Infrared Measurements of Precursor Radiation in the X2 Expansion Tube

S. G. Lock[1,a)], Y. Liu,[1], T. J. McIntyre[2], R. G. Morgan[1] and C. M. James[1]

[1]*Centre for Hypersonics, School of Mechanical and Mining Engineering, The University of Queensland.*
[2]*Centre for Hypersonics, School of Mathematics and Physics, The University of Queensland.*

[a)]Corresponding author: samuel.lock@uq.net.au

For spacecraft re-entering Earth's atmosphere on sample or Mars return trajectories, radiation, over convection, is expected to become the dominant form of heat transfer to the vehicle [1]. Accurate modelling and prediction of the post-shock environment in these radiation dominated flows requires detailed consideration of radiation coupling mechanisms, one of which being precursor radiation. Precursor radiation occurs in the presence of a strongly radiating shock layer, through which downstream post-shock radiation can change the chemical composition and temperature of the upstream gas by means of photoionisation, photodissociation, and photoexcitation.

Despite altering the state of the free-stream, the influence of precursor radiation on the post-shock flow and heating environment remains an open area of research. Stanley et al. [2] modelled the effect of precursor radiation for a 15 km/s Mars return condition in a nitrogen atmosphere, concluding that, despite significant changes to the freestream composition and temperature the phenomena had a negligible effect on the post-shock environment. Contrastingly, the work by Johnston et al. [3] found that for a 15 km/s re-entry condition, the precursor radiation effect not only brought freestream vibrational-electronic temperatures to their post-shock values, but increased the post-shock temperatures by approximately 150 K. Given the sensitivity of radiative emission to temperature, this small increase in post-shock temperature was found to increase the wall radiative flux by 15%. As such, there remain large uncertainties surrounding the effect of precursor radiation for high speed Earth re-entry conditions.

Several experimental campaigns have been undertaken investigating the phenomena, especially given its early importance in the study of communications blackout. Early experiments took the form of microwave interferometry, whereas more recent work has mostly focused on the use of Langmuir probes in shock tube environments to study the photoionisation in front of shock layers [4]. These experiments highlighted discrepancies between existing numerical models, and emphasised the need for an in-depth understanding of the underlying processes and need to use iterative coupled numerical techniques when modelling these flows [5, 6]. Yamada et al. [7] utilised a photomultiplier tube to capture time-resolved emission spectroscopy measurements over a narrow wavelength region for molecular and atomic nitrogen. Despite measuring the relatively slower shock velocities of 6 km/s, they also observed significant levels of nitrogen radiation present in the precursor region. Vacuum-ultraviolet (VUV) shock layer radiation measurements in the X2 expansion tube facility have also shown evidence of radiation in the precursor region [8], however the study also suggested further investigation to rule out the possibility that it was caused by factors such as contaminants or unsteady shock effects. The majority of those targeted precursor studies have focused on measurements in shock tube facilities, studying electron number density and temperature distributions ahead of moving shock waves. The use of an expansion tube, however, overcomes restrictions associated with a moving shock by observing the quasi-steady shock layer and precursor region formed over a model. An additional benefit is the increase in test time these facilities enable, allowing for longer exposure times and higher signal measurements of the precursor region when using techniques such as broadband emission spectroscopy.

For this study, emission spectroscopy was used in the X2 expansion tube facility to study the shock layer and precursor radiation associated with a 13 km/s Earth re-entry over a truncated 40mm radius, 80mm long cylindrical model. Radiation measurements were acquired simultaneously from the VUV to the near-infrared spectral regions. Whilst the line-of-sight of the spectral system was fixed, the precursor region was probed by moving the model, originally setback 353 mm from the line-of-sight, incrementally forward.

REFERENCES

[1] J. S. Robinson, K. E. Wurster, J. C. Mills, *Journal of Spacecraft and Rockets* **46**, 74–861 (2009).
[2] S. A. Stanley, L. A. Carlson, *Journal of Spacecraft and Rockets* **29**, 190–1973 (1992).
[3] C. O. Johnston, A. Mazaheri, P. Gnoffo, B. Kleb, D. Bose, *Journal of Spacecraft and Rockets* (American Institute of Aeronautics and Astronautics Inc., 2013), 19–38.
[4] K. Fujita, S. Sato, T. Abe, A. Matsuda, *35th AIAA Thermophysics Conference* (American Institute of Aeronautics and Astronautics, 2001).
[5] A. Lemal, S. Nomura, H. Takayanagi, K. Fujita, *2018 AIAA Aerospace Sciences Meeting* (American Institute of Aeronautics and Astronautics, 2018).
[6] S. Nomura, T. Kawakami, K. Fujita, *Journal of Thermophysics and Heat Transfer* **35**, 518–5237 (2021).
[7] G. Yamada, M. Kajino, K. Ohtani, *Journal of Fluid Science and Technology* **14**, JFST0022–JFST0022 (2019).
[8] U. A. Sheikh, R. G. Morgan, T. J. McIntyre, *AIAA Journal* **54**, 2407–24175 (2016).

A Comparative Assessment of Moment-Based Closures for Flows at Various Levels of Rarefaction

D. Biasone[1,2,a)], P. Bernigaud[1] and M. Massot[2]

[1]*DMPE, ONERA, Université Paris Saclay, 91120 Palaiseau, France*
[2]*CMAP, CNRS, École polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France*

[a)]Corresponding author: daniele.biasone@polytechnique.edu

Many engineering applications require accurate representation of flows with spatially varying degrees of rarefaction. A representative example is given by high-altitude rocket engine plumes, where the gas expansion through the nozzle transitions from dense combustion-chamber conditions to highly rarefied flow in the low-pressure ambient atmosphere. In such cases, usual techniques struggle to provide effective predictions. In fact, stochastic methodologies, such as Direct Simulation Monte Carlo (DSMC), require the time step and cell size to be smaller than the particle collision time and mean free path, respectively. These requirements result in prohibitive computational costs in dense regions of the flow. On the other hand, conventional Computational Fluid Dynamics (CFD) techniques, based on the Navier-Stokes equations, suffer from a loss of accuracy due to the breakdown of the underlying continuum assumptions, thus making them unable to capture non-equilibrium effects in rarefied regions. In recent years, hybrid methods that blends CFD and DMSC solvers have been developed [1]. The flow field is decomposed into continuum and rarefied regions: the first portion is solved using CFD, while the rarefied domain is handled with DSMC, with the two solvers being coupled through a user-defined interface [2, 3]. Although such hybrid strategies have reached a high level of maturity, their main challenge remains the definition of the coupling interface, whose placement can strongly affect the solution [4, 5].

A promising alternative is offered by the method of moments. By taking velocity moments of the Boltzmann equation, this framework generates a hierarchy of conservation equations for macroscopic quantities that incorporate non-equilibrium effects. Nevertheless, this hierarchy is infinite, and must be truncated for practical applications. Truncation, however, leads to an underdetermined system due to the presence of unknown fluxes, which requires the introduction of an appropriate closure relation, typically formulated as an assumption on the functional form of the local distribution function. Whereas various closures for moment equations have been proposed, a complete investigation of their capabilities in resolving rarefied flow fields is still an open question. The present work aims at providing an in-depth comparison between different existing closure strategies, including Grad-type closures [6, 7], maximum entropy approaches [8, 9], and quadrature-based methods [10, 11], evaluating their performance in capturing rarefied flows over a wide range of rarefaction levels with BGK collisions. The methods are compared against reference solutions obtained by the Discrete Velocity Method. Closure strategies are analysed in terms of accuracy, robustness and computational cost. Particular emphasis is placed on the structural properties of the various methods, in particular realizability and preservation of hyperbolicity, and on how these properties affect the reconstruction of the main characteristics of the cases under examination. The results offer guidelines for selecting suitable closure strategies based on flow conditions and computational requirements.

ACKNOWLEDGEMENTS

The authors would like to acknowledge the financial support from ONERA and from the Agence Innovation Défense (AID) within the CIEDS project OPEN-NUM-DEF (PI: L. Gouarin, M. Massot, T. Pichard).

REFERENCES

[1] T. Schwartzentruber, I. Boyd, *Journal of Computational Physics* **215**, 402–416 (2006).
[2] F. La Torre, S. Kenjereš, J.-L. Moerel, C. Kleijn, *Computers & Fluids* **49**, 312–322 (2011).
[3] A. Clout, A. Langenais, Y. Dauvois, L. Mieussens, J. Labaune, *Physics of Fluids* **37**, 016119 (2025).
[4] K. Xu, J.-C. Huang, *Journal of Computational Physics* **229**, 7747–7764 (2010).
[5] V. Charton, A. Awad, J. Labaune, *Acta Astronautica* **195**, 295–308 (2022).
[6] H. Grad, *Communications on Pure and Applied Mathematics* **2**, 331–407 (1949).
[7] Z. Hu, Z. Cai, Y. Wang, *SIAM Journal on Scientific Computing* **42**, B105–B134 (2020).
[8] C. D. Levermore, *Journal of Statistical Physics* **83**, 1021–1065 (1996).
[9] M. R. A. Abdelmalik, E. H. van Brummelen, *Journal of Statistical Physics* **164**, 77–104 (2016).
[10] C. Chalons, R. Fox, M. Massot, *Proceedings of the Summer Program* (Center for Turbulence Research, Stanford University, 2010), 347–358.
[11] R. O. Fox, F. Laurent, *SIAM Journal on Applied Mathematics* **82**, 750–771 (2022).

Abstract 163

Monte Carlo modeling of nonstoichiometry in laser produced plasmas of a binary alloy target

Rommil B. Emperado[1,a)], Arjay M. Dulay[1], Marc Robert R. Casero[1], Myles Allen H. Zosa[2], Lean L. Dasallas[1], and Wilson O. Garcia[2]

[1] *Materials Science and Engineering Program, College of Science, University of the Philippines Diliman, Quezon City, Philippines, 1101*
[2] *National Institute of Physics, University of the Philippines Diliman, Quezon City, 1101*

[a)] Corresponding author: rbemperado@up.edu.ph

Shining a high-powered pulsed laser on a target leads to the formation of laser-produced plasmas (LPPs) with compositions that generally match that of the irradiated material, allowing for applications in characterization [1] and thin film deposition [2]. However, the plume is nonstoichiometric in some cases because of incongruent evaporation and separation of species during flight towards the substrate [3]. Optimizing the plume stoichiometry is essential for film deposition applications but remains to be an open problem [4], and the spatiotemporal separation of binary plume species in a background gas has not been modeled yet via DSMC to the best of our knowledge. Here, we used the open-source code SPARTA to model in 3D the expansion of AuCu LPP in neon gas and the spatiotemporal evolution of the number density of the plume and gas species along with the LPP flux through planes at 5 mm, 10 mm, and 15 mm away from the target. In vacuum, Cu propagates faster than Au near the target, but the stoichiometry improves as the plume reaches the 15 mm substrate. This is also observed for LPPs in 0.1 mbar, 0.5 mbar, and 2 mbar Ne gas. Increasing the gas pressure normally improves the stoichiometry; however, the formation of a high-density gas region and shock wave [5, 6] in between the substrate and incoming plume leads to more collisions between plume species, resulting in Au-poor deposition to the substrate. This study highlights not just the spatiotemporal expansion of binary plume species but also the influence of shock wave formation on the stoichiometry of deposited films.

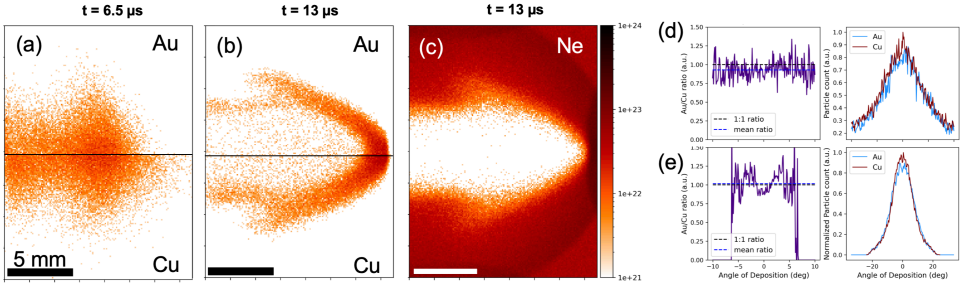


Fig. 1. (a, b) Number densities of Au and Cu in vacuum and in 2 mbar Ne gas at 6.5 ms and 13 ms, respectively, along with (c) the corresponding number density of 2 mbar Ne background gas. (d, e) Au/Cu ratio and thickness profile for LPP expansion in vacuum and 2 mbar Ne gas, respectively.

ACKNOWLEDGEMENTS

This work is supported by the University of the Philippines Diliman Natural Sciences Research Institute (Project No. MSE-26-1-02). We also acknowledge the National Institute of Physics, U.P. Diliman for the computational resources.

REFERENCES

[1] L. Brunnbauer, Z. Gajarska, H. Lohninger, A. Limbeck, *Trends in Analytical Chemistry*, **159**, p. 116859 (2023).
[2] L. Duta, A. C. Popescu, *Coatings*, **11**(3), p. 274 (2021).
[3] S. Canulescu, M. Döbeli, X. Yao, T. Lippert, S. Amoruso, J. Schou, *Physical Review Materials*, **1**(7), p. 073402 (2017).
[4] A. A. Morozov, S. V. Starinskiy, A. V. Bulgakov, *Journal of Physics D: Applied Physics*, **54**(17), p. 175203 (2021).
[5] A. N. Volkov, Z. Lin, *International Journal of Heat and Mass Transfer,* **216**, p. 124511 (2023).
[6] R. B. Emperado, M. A. H. Zosa, L. L. Dasallas, W. O. Garcia, *Physics of Fluids*, **37**(3) (2025).

Non-Equilibrium Applications of Hyperbolic Higher-Order Moment Models with Solid-Wall Boundary Conditions

E. D. Rice[*1], S. Boccelli[2] and J. G. McDonald[1]

[1] *University of Ottawa, Department of Mechanical Engineering, 161 Louis Pasteur, Ottawa, ON, Canada*
[2] *NPP Postdoctoral Fellow, NASA Goddard Space Flight Center, 8800 Greenbelt Rd, Greenbelt, MD, United States*

[*]Corresponding author: erice033@uottawa.ca

Moment closures of gas kinetic theory are an increasingly popular method for rarefied gas flow prediction. In the transition regime where the continuum assumption is invalid, but interparticle collisions are still relevant, there is a lack of robust and efficient models. In this regime, continuum assumption based models like the Navier-Stokes equations give physically inaccurate predictions, while particle based methods like direct simulation Monte Carlo (DSMC) are significantly more computationally expensive. Moment closures offer a way to extend traditional CFD techniques into this regime. Although traditional moment closures propose distribution functions for the behavior of gas particles, recent works [1–4] have focused on the partial differential equations that arise from the problem of moment closure itself instead. This has allowed for the development of hierarchies of robustly hyperbolic moment closures that are in a highly desirable balance-law form. However, use of moment models in non-equilibrium settings remains underexplored. As a consequence of avoiding the prescription of a known distribution function, the formulation of solid-wall boundary conditions remains an open question to address in the context of these new models.

This work presents a review of these new moment closure methods, including the robustly hyperbolic 20-moment model. Following a review of the traditional Knudsen-layer approximation for moment closures with known distribution functions, a modification of Steger-Warming flux splitting is proposed as a hyperbolic characteristic-based approximation of the required half-space integrals. Results for simple planar flows across the regimes of interest for moment methods with this new boundary condition treatment, including Couette flow and heat transfer between plates, are investigated and compared against known solutions for these simple cases. To demonstrate the robustness and resolution capabilities of the 20-moment model, as well as the consistency and stability of the new formulation for boundary conditions, multidimensional flows are explored in both the continuum and transition regimes. These are shown in comparison with their more computationally expensive counterparts. One of these cases, transonic Mach 0.95 flow past a fully accommodated cylinder at a Knudsen number of 0.1, is shown in Figures 1 and 2. Figure 1 shows the density profile of both solutions, where the 20-moment model resolves a sharper density gradient over the top of the cylinder, while the DSMC solution exhibits significant statistical noise that obscures the shock structure. To characterize non-equilibrium regions, Figure 2 shows the condition number of the temperature tensor. Although areas of low temperature anisotropy are captured similarly between both models, the 20-moment model produces more spatially coherent anisotropic structures, while the DSMC result exhibits statistical fluctuations in these regions. Other flows with large regions of non-equilibrium, and future extensions (e.g., diatomic gases and plasmas), conclude the presentation.

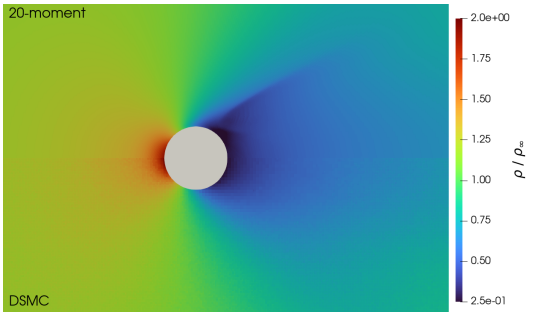


Fig. 1. Comparison of 20-moment and DSMC predicted density profiles

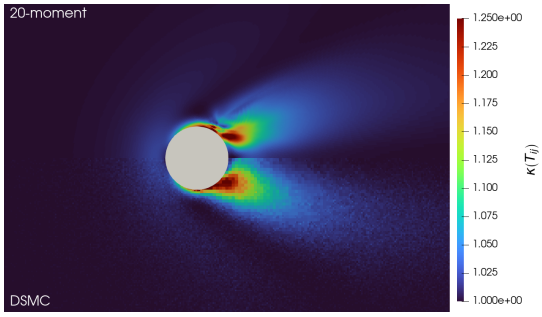


Fig. 2. Comparison of 20-moment and DSMC predicted temperature anisotropy profiles

REFERENCES

[1] R. O. Fox, F. Laurent, *SIAM Journal on Applied Mathematics* **82**, 750–771 (2022).
[2] W. Morin, J. G. McDonald, *Journal of Computational Physics* **523**, 113659 (2024).
[3] L. Bell, H. Struchtrup, *Physics of Fluids* **37**, 067122 (2025).
[4] E. Rice, J. G. McDonald, *Journal of Computational Physics (Accepted pending revisions)* (2026).

Symmetrizable Hyperbolic Moment Closures with a Convex Entropy

B. Allard[1,a] and J. G. M^{c}Donald[1]

[1] *University of Ottawa, Department of Mechanical Engineering, 161 Louis Pasteur, Ottawa, ON, Canada*

[a] Corresponding author: benoit.allard@uottawa.ca

Moment methods derived from the Boltzmann equation provide a systematic route from kinetic theory to tractable continuum systems by evolving a finite set of moments. The central challenge is closure: truncation must supply higher-order constitutive information of higher-order moments while preserving structural properties, notably global hyperbolicity. Standard strategies include Grad-type polynomial expansions [1], quadrature-based moment methods (QMOM) [2, 3], and entropy-based closures from maximum-entropy / extended-thermodynamics principles [4, 5]. Entropy-based closures are attractive due to their primal-dual structure: a convex density potential, $h(\boldsymbol{\alpha})$, generates the moment map and provides a symmetrizer. However, for higher-order systems this approach is often computationally prohibitive because it requires repeatedly solving a nonlinear optimization problem for the entropy variables, $\boldsymbol{\alpha}$, at every space-time point.

We explore a broader design space for density potentials beyond standard exponential-integral ansätze by representing $h(\boldsymbol{\alpha})$ as a finite sum of exponential–polynomial modes. We derive constraints on the mode parameters such that $\nabla^2 h$ is a (semi-)positive definite Hankel moment matrix, yielding a convex extension and therefore a hyperbolic, symmetrizable closed moment system. We identify several admissible families, including single-phase families (modes depending on a single scalar phase in $\boldsymbol{\alpha}$-space) and fixed-mode ($\boldsymbol{\alpha}$-independent stencil) families, e.g., [6]. For instance, the compressible Euler equations emerge as a degenerate single-phase closure within this framework. Fixed-mode families are straightforward to compute because the associated entropy-variable inversion remains convex on a prescribed exponential stencil, but they are limited by the q-realizability [7] region accessible to that stencil. An example of a 4-moment closure solution to a one-dimensional stationary Mach 2 shock is illustrated in Fig. 1. However, we outline ongoing efforts at extending the single-phase construction to higher-order in a way that expands realizable moment space while preserving symmetrizable hyperbolicity.

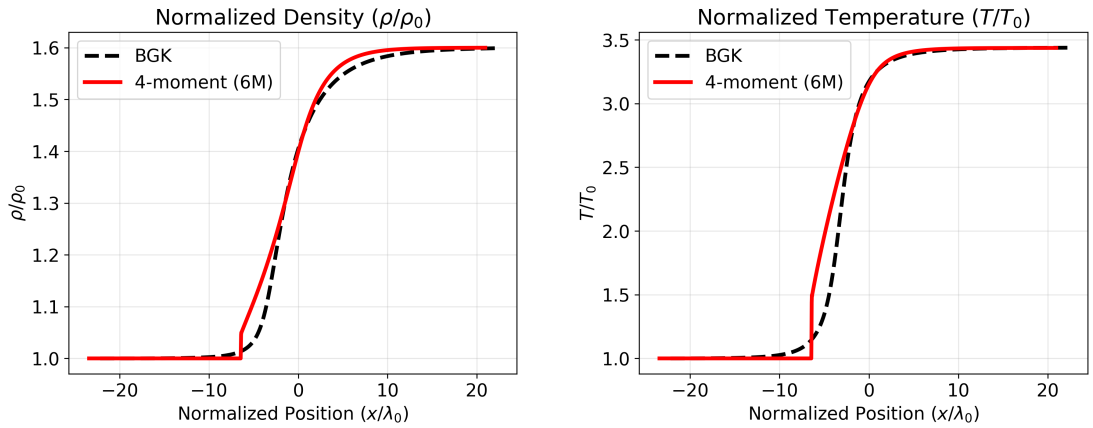


FIGURE 1. Comparison of a 4-moment (6) fixed-mode closure and exact BGK solution to a one-dimensional stationary Mach 2 shock.

REFERENCES

[1] H. Grad, *Communications on Pure and Applied Mathematics* **2**, 331–407 (1949).
[2] R. McGraw, *Aerosol Science and Technology* **27**, 255–265 (1997).
[3] R. Fox, F. Laurent, *SIAM Journal on Applied Mathematics* **82**, 750–771 (2022).
[4] C. Levermore, *Journal of Statistical Physics* **83**, 1021–1065 (1996).
[5] I. Müller, T. Ruggeri, *Rational Extended Thermodynamics* (Springer, New York, NY, 1998).
[6] R. Schaerer, M. Torrilhon, *European Journal of Mechanics - B/Fluids* **64**, 30–40 (2017).
[7] G. Alldredge, C. Hauck, D. OLeary, A. Tits, *Journal of Computational Physics* **258**, 489–508 (2014).

Abstract 169

A Kinetic Linear Stability Theory Framework for High Speed Flows

I. T. Karpuzcu[1,a)], M. Aharoni[2], **D. A. Levin[1]**, and V. Theofilis[2]

[1] *University of Illinois Urbana-Champaign IL 61801 USA.*
[2] *Technion - Israel Institute of Technology, Haifa 32000, Israel.*

[a)] Corresponding author: itk3@illinois.edu

We present the development and implementation of a high-fidelity kinetic linear stability theory (kLST) framework designed for compressible high-speed flows. Traditional stability theories rely on the Navier-Stokes equations, which fundamentally break down in the presence of strong shock waves and highly rarefied regimes. To accurately capture the translational non-equilibrium effects prevalent in these shock-dominated flows, our methodology directly linearizes the Boltzmann equation using the Bhatnagar-Gross-Krook (BGK) collision operator, thus solving for the perturbations directly in the velocity distribution function. We have established a robust parallel computational framework that utilizes Gauss-Hermite quadrature for velocity space discretization and Chebyshev collocation for spatial derivatives. The resulting large-scale generalized eigenvalue problem is efficiently processed using sparse matrix techniques, an Arnoldi eigenvalue solver, and a shift-and-invert transformation via the SLEPc/PETSc framework. The developed kLST solver is first rigorously verified against continuum compressible Couette flow, demonstrating excellent agreement with established Navier-Stokes-based eigenvalue spectra for varied Mach numbers and wavenumbers **[1]**. The framework is subsequently extended to analyze the stability of one-dimensional normal shocks. Our modal stability analysis reveals that even moderate departures from thermal equilibrium intrinsically alter the flow's stability characteristics, inducing measurable shifts across the entire eigenvalue spectrum and rendering the flow globally less stable than equilibrium considerations. These findings demonstrate the critical importance of incorporating kinetic-level physics into stability analysis, verifying this framework as a scalable and essential tool for predicting instability and transition in canonical hypersonic configurations.

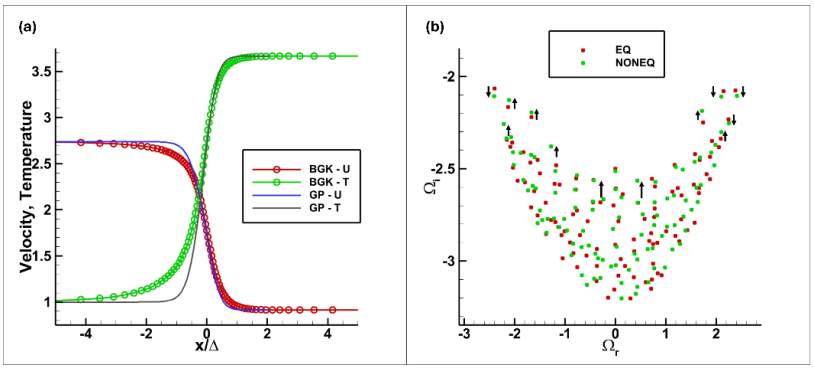


Figure 1. (a) Shock profiles for a Argon flow at M=3 and (b) eigenvalue spectra for kLST results using equilibrium and non-equilibrium velocity distribution functions.

ACKNOWLEDGEMENTS

Research supported by the Office of Naval Research under Grant No. N00014-23-1-2839 titled “Kinetic Treatment of Sources and Mechanisms that Drive Unsteady, Shock-dominated Flow Instability”.

REFERENCES

[1] Zou, S., Bi, L., Zhong, C., Yuan, X., and Tang, Z., “A normal-mode approach for high-speed rarefied plane Couette flow,” *Physics of Fluids*, Vol. 36, No. 1, 2024, p. 014121.
[2] Gilbarg, D., and Paolucci, D., “The Structure of Shock Waves in the Continuum Theory of Fluids,” *Journal of Rational Mechanics and Analysis*, Vol. 2, 1953, pp. 617–642.

Abstract 170

MD-DSMC modelling of gas-surface interaction for VLEO systems.

S. Nair[1,a)], A. Appar[2], and S. Poovathingal[1]

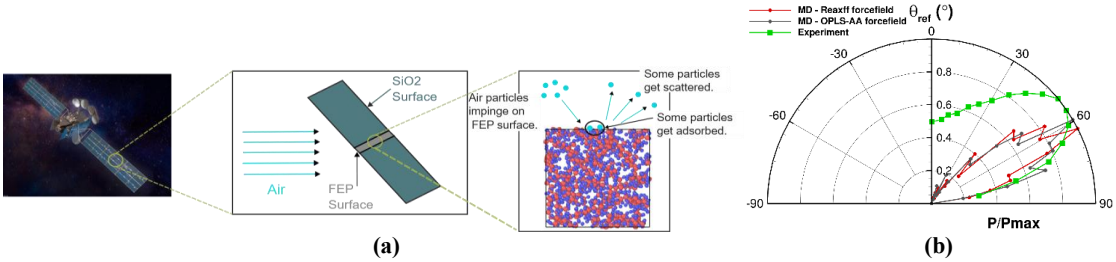
[1]*Department of Mechanical and Aerospace Engineering, University of Kentucky, 351 Ralph G. Anderson Building, Lexington, KY 40506-0503, USA.*
[2]*Department of Aerospace Engineering, Universidad Carlos III de Madrid (UC3M), Escuela Politécnica Superior, Avda. de la Universidad, 30. 28911 Leganés, Madrid, Spain.*

[a)] Corresponding author: sna328@uky.edu

Over the past five years, the number of active satellites in orbit has more than quadrupled, which has led to increased congestion in the traditional Low Earth Orbit (LEO). Very Low Earth Orbit (VLEO), altitude regime below LEO (250 - 450 km), is emerging as a preferred alternative because of lower launch costs, reduced traffic, and self-cleaning nature [1]. However, satellites operating in VLEO encounter significantly higher drag because of increased atmospheric density at those altitudes. Our work aims to develop first principles based molecular dynamics (MD) and direct simulation Monte Carlo (DSMC) gas-surface interaction (GSI) models for accurately predicting aerodynamic drag on VLEO satellites (Fig. 1a). Fluorinated Ethylene Propylene (FEP) Teflon is chosen as our target material, which is mostly used as a glue on satellites.

A fundamental challenge to overcome in MD simulations is surface preparation. Thousands of FEP polymer chains are randomly placed inside a box and subjected to a sequence of NVT and NPT ensemble relaxation steps at 300 K to produce a stable amorphous bulk structure. OPLS-AA forcefield is utilized with fixed, unbreakable bonds to generate a stable structure at the desired density. After structure preparation, scattering of oxygen atoms is studied. A series of atomic oxygen particles are impinged onto the FEP Teflon slab, and the angular distribution of the scattered atoms are generated and compared against atomic oxygen beam scattering experiments [2]. In one simulation, a single oxygen atom is introduced 10 Å above the slab and is impinged with an incident kinetic energy of 5 eV (0.078 Å/fs). These individual scattering simulations are repeated 5000 times, with the oxygen atom initialized at randomly sampled x and y starting positions above the slab surface to obtain statistically meaningful scattering distributions. Both OPLS-AA and ReaxFF forcefields are tested. For an incident angle of 60º, the scattering angle distributions obtained using ReaxFF and OPLS-AA show good agreement (Fig. 1b), however, the MD-predicted distributions demonstrate poor agreement with experimental observations.

Our next objective is to incorporate roughness effects in scattering to assess multiple collisions of O atoms on the surface. This meso-scale phenomenon will be modeled using DSMC technique.



(a) **(b)**

Fig. 1 (a) GSI Illustration on satellites. (b) Scattering angle distribution.

ACKNOWLEDGEMENTS

The material is based upon the work supported by the DARPA Young Faculty Award #D24AP00309 to Poovathingal. The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of DARPA or the U.S. Government.

REFERENCES

[1] N. H. Crisp. et al. *Progress in Aerospace Sciences*, 117, 100619 (2020).
[2] C. Xu. et al. *CEAS Space Journal.* (2025), *https://doi.org/10.1007/s12567-025-00628-5.*

Abstract 171

Parametric Velocity Modes from DSMC Shocks

R. S. Martin[1,a)]

[1] *DEVCOM Army Research Office, 800 Park Offices Dr., Research Triangle Park, NC, USA*

[a)] Corresponding author: robert.s.martin163.civ@army.mil

In Ref [1], it was shown that relatively low dimensional orthogonal velocity distribution function modes could be extracted from 1D Direct Simulation Monte Carlo (DSMC) normal shock wave simulations if the distributions were first centered and scaled using the pointwise distribution mean velocity and temperature. The Mach 2 shock required only 3 additional perturbation modes and Mach 8 only 7 modes to capture the significant distribution deviations above the noise floor. However, for development of a global reduced order model (ROM) basis suitable for a wide range of normal shock waves, there should be an expectation that the modes included in the global basis are sufficient to accurately represent the distribution throughout the parametric range of shock strengths. In the case of the prior study, the 3 modes at Mach 2 were not well representable by the 7 Mach 8 modes, implying a large angle between the subspaces as described in Ref [2].

In this work, shock modes will be extracted from a finer range of normal shocks. An initial array of cases is shown in Fig. 1. This initial array will be used to determine how rapidly the modal subspace shifts as a function of Mach number to determine where additional refinement or coarsening may be warranted. This will shed light on whether building a single global basis capable of spanning weak to strong normal shocks is viable, or if the required number of basis functions to span the parametric subspace to high accuracy would lead to a prohibitively expensive precomputation of the Boltzmann collision integrals as described in Ref [3]. The work will also consider the impact of variable hard-sphere coefficient corresponding to the viscosity index ranging from a hard sphere model though the monatomic gasses Helium, Argon, and Xenon through the Maxwell model as a second dimension of parametric dependence for the velocity distribution modes. While this will still not support ROMs of multispecies mixtures where velocity distributions deviate more significantly from equilibrium, this will help determine if a single pure gas ROM can be developed for a range of gasses with differing viscosity scaling laws.

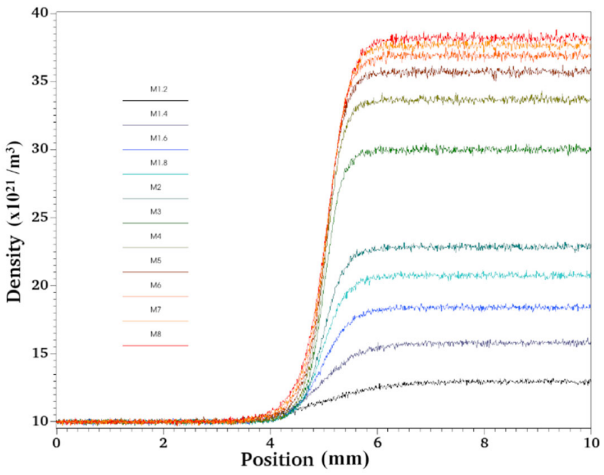


Fig. 1. Initial array of steady-state Argon normal shock instantaneous number densities for initial upstream temperature of 293K.

The implied complexity of the resulting ROMs will then be discussed in the context of the learned closure problem of Ref [4]. This will shed light on what level of moment method can be conceptually expected to close with local state and gradient information for a bounded class of single species normal shock problem.

ACKNOWLEDGEMENTS

This work was supported in part by high-performance computer time and resources from the DoD High Performance Computing Modernization Program.

REFERENCES

[1] R.S. Martin, (to appear) *Proc. of the 33rd Int. Symp. Rarefied Gas Dynamics*, (2026).
[2] A. Mohaghegh and C. Huang, *AIAA SciTech Forum,* (2026).
[3] A. Alekseenko, R. S. Martin, A. Wood, *J. Comp. Phys.,* **470**, 111526, (2024).
[4] G. Garg, T.K. Mankodi, E. Esmaeilifar, and R.S. Myong, *Phys. Fluids,* **36**, 106113, (2024).

DISTRIBUTION STATEMENT A: Approved for Public Release. Distribution is Unlimited.

Investigation of Thermochemical Effects on Hypersonic Flow Unsteadiness Over a Double Cone

S. Thirani[1,a)] and **D. A. Levin**[1]

[1]*Department of Aerospace Engineering, University of Illinois, Urbana-Champaign, IL, USA.*

[a)]Corresponding author: thirani2@illinois.edu

The canonical case of hypersonic flow over a double cone provides an avenue to investigate complex shock interactions with a boundary layer. Experiments conducted in the CUBRC facility [1] obtained measurements of surface parameters, such as heat flux and pressure, for a hypersonic oxygen flow over a 25°/55° double cone geometry. As part of this work, we will use the Direct Simulation Monte Carlo (DSMC) [2] method to investigate the effect of thermochemistry on flow unsteadiness over the double cone for the experimental conditions of the CUBRC experiments while utilizing the nonequilibrium thermochemistry models described by Gimelshein and Wysong [3]. The geometry and test conditions from the experiments have been studied with particle methods by Valentini et al. [4] who achieved reasonable agreement between simulations and experimental measurements for surface parameters. Tumuklu et al. [5] studied the geometry for pure N2 flows at a higher Mach number and reported the presence of unsteady modes in the flow.

Preliminary result presented in Fig. 1 shows contour plots of the magnitude of density gradient for the case where dissociation of O_2 was included in the thermochemistry modeling. The plot highlights flow structures such as the separation shock, triple point, transmitted shock, detached shock and separation bubble. Figure 2 presents comparisons of probe data for pressure near the triple point for calculations including and without including the reactions for O_2 dissociation in the thermochemistry modeling. We observe that the inclusion of O_2 dissociation leads to slower decay rates for the initial pressure unsteadiness in comparison to the calculation that did not include O_2 dissociation. The authors are working on post-processing time accurate snapshots of the flowfield using the dynamic mode decomposition technique to identify global eigen modes in the flowfield, and will be presenting their findings at the symposium.

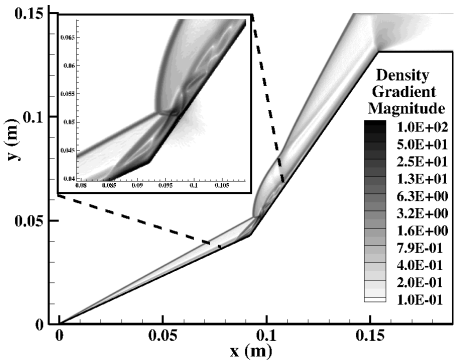


Fig. 1. Density gradient magnitude for case with dissociation.

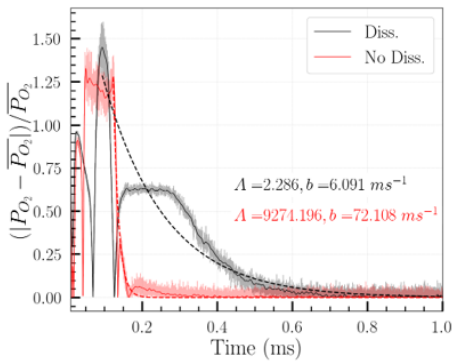


Fig. 2. Pressure unsteadiness near triple point.

ACKNOWLEDGEMENTS

The research is being performed at the University of Illinois Urbana-Champaign and is supported by the Air Force Office of Scientific Research through AFOSR Grant No. FA9550-25-1-0225. Computational resources for this research are provided by the National Science Foundation TACC's Stampede3 supercomputer, which is a part of ACCESS, with the project number TG-PHY220158.

REFERENCES

[1] M. Holden, *38th Aerospace Sciences Meeting and Exhibit* (2000).
[2] G. A. Bird, in *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Clarendon, Oxford, England, U.K., 1994).
[3] S. F. Gimelshein, I. J. Wysong, *Physical Review Fluids* **4**, 033405 (2019).
[4] P. Valentini, M. S. Grover, A. M. Verhoff, N. J. Bisek, *Journal of Fluid Mechanics* **966**, A32 (2023).
[5] O. Tumuklu, V. Theofilis, D. A. Levin, *Physics of Fluids* **30**, 106111 (2018).

Modeling reflected-shock tube experiments using *ab initio* vibrational specific kinetics for oxygen mixtures

L. F. Rodriguez[1,a)] and R. L. Macdonald[1]

[1]*Aerospace Engineering Sciences, University of Colorado Boulder, CO, 80303, USA.*

[a)]Corresponding author: luro8836@colorado.edu

Shock waves in hypersonic flows convert kinetic energy into thermal energy, promoting internal excitation of particles and driving chemical reactions. Thermochemical nonequilibrium persists over timescales comparable to the characteristic flow convection time. Reflected–shock experiments provide a controlled environment for isolating and validating nonequilibrium kinetic models, as the post–reflected–shock gas is nearly stagnated in the laboratory frame while undergoing thermochemical relaxation. This work presents a modeling framework developed to reproduce and interpret reflected–shock experiments in pure oxygen conducted at Stanford by Hanson's group. The simulations employ a one–dimensional steady–state shock solver implemented within the PLATO library. Reflected–shock conditions are modeled using a three–step space–marching methodology that accounts for (i) incident–shock relaxation, (ii) reflected–shock deceleration through end–wall boundary conditions, and (iii) flow evolution at the measurement location [1]. Vibrationally resolved kinetics are incorporated using a reduced database derived from quasi–classical trajectory (QCT) calculations based on *ab initio* potential energy surfaces (PESs) developed by Paukku et al. [2]. The present model incorporates Mirels effects through source terms in the momentum and energy conservation equations, using the experimentally measured pressure rise (dP/dt) at the observation location[3].

The Park two-temperature (2T) model and the QCT-based vibrational kinetics model were implemented within the present three-step marching framework, incorporating the multisurface correction factor of 16/3 for dissociation reactions. Figure 1 shows that both models deviate from the experimental data reported by Streicher *et al.*[3], underpredicting and overpredicting the experimental equilibrium temperatures, respectively. In contrast, the Modified Marrone–Treanor (MMT) model implemented within the same methodology by Aiken[1] shows good agreement with the experimental data, particularly near equilibrium. The final phase of this work aims to investigate the origin of the deviations between the experimental measurements and the vibrational-kinetics predictions. Particular attention will be given to potential inconsistencies in the source-term implementation, fitting inaccuracies in the bound–bound rate coefficients—especially when using non-Arrhenius functional forms as proposed by Baluckram et al. [4]—and the development of a simplified, physically informed representation of the Mirels effect.

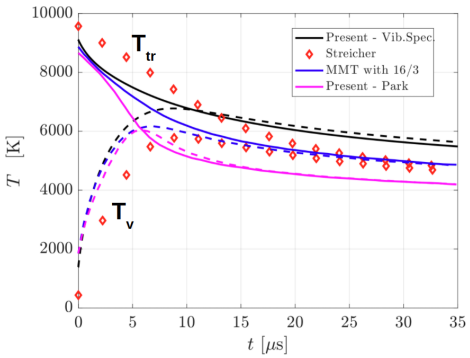


Fig. 1. Predicted T_{tr} and T_v relaxation behind the reflected shock using 2T and vibrational kinetics models.

ACKNOWLEDGEMENTS

This work has been funded by the Office of Naval Research (ONR), through the Multidisciplinary University Research Initiatives (MURI) Grant N00014-22-1-2661. This work utilized the Blanca condo computing resource at the University of Colorado Boulder. Blanca is jointly funded by computing users and the University of Colorado Boulder.

REFERENCES

[1] T. T. Aiken, I. D. Boyd, Journal of Thermophysics and Heat Transfer **37**, 723–732 (2023).
[2] Y. Paukku, Z. Varga, D. G. Truhlar, The Journal of chemical physics **148** (2018).
[3] J. W. Streicher, A. Krish, R. K. Hanson, Physics of Fluids **32** (2020).
[4] V. T. Baluckram, A. J. Fangman, D. A. Andrienko, Journal of Thermophysics and Heat Transfer **37**, 198–212 (2023).

Influence of diffusion modelling on catalytic wall heat flux in hydrogen/helium boundary layers

M. Uren[1,a)], Y. Liu,[1], C. M. James[1] and R. G. Morgan[1]

[1]*Centre for Hypersonics, School of Mechanical and Mining Engineering, The University of Queensland, St Lucia, QLD, 4072, Australia.*

[a)]Corresponding author: matthew.uren@uq.edu.au

Over the history of human spaceflight, no dedicated mission has ever been sent to the ice giant planets, Uranus and Neptune. Due to their high potential for scientific value, an ice giant orbiter and probe mission has been highlighted as high priority by NASA in the 2022 Decadal Survey [1]. The atmospheric entry environment of the ice giants differs considerably from Earth re-entry and introduces new challenges and uncertainties outside of the realms of existing expertise. Ice giant entry velocities are predicted to be on the order of 20 km/s to 30 km/s, well beyond the limits for Earth re-entry. Furthermore, the atmospheric compositions are composed primarily of molecular hydrogen, with smaller fractions of helium and trace species such as methane. Research effort in this area has increased over the past decade on obtaining more experimental data in appropriate ground testing facilities, and increasing the fidelity of numerical simulations to more accurately predict the entry environment.

The thermal loading during ice giant entry is generally considered to be dominated by convective heating, with radiative heating becoming influential at higher entry velocities, particularly for Neptune [2]. The magnitude of the convective heat flux is believed to be strongly influenced by species diffusion and the recombination rate of H2 within the boundary layer [2]. Uncertainties in the rates for each mechanism can lead to order of magnitude variations in the predicted wall heat flux, becoming even more prevalent when the surface is partially catalytic. A study into proposed ice giant aerocapture mission trajectories also identified the collision integrals and transport coefficients as being a driver of uncertainty for heat flux if the wall surface is partially catalytic [3].

The heat transfer across a hypersonic boundary layer can be largely dependent on the chemical state of the flow arriving at the wall. When the rate of diffusion is greater than the recombination rate of dissociated species through the boundary layer, then the boundary layer will be chemically frozen. Under these conditions, a high concentration of dissociated species reaches the wall, and the potential for surface heat flux by recombination at the wall is maximised. The choice of diffusion model directly impacts the boundary layer Damköhler number and therefore the available chemical potential energy at the wall that can augment surface heating. Diffusion is therefore the rate-governing mechanism for surface heat transfer in boundary layers that are in chemical non-equilibrium [4].

This study investigates how sensitive the predicted heat flux on a catalytic wall is to the choice of diffusion model in high enthalpy hydrogen/helium boundary layers, representative of ice giant entry flows. An initial parametric study to ascertain the influence of the diffusion coefficient on heat flux under varying catalytic wall boundary conditions will be undertaken using a reduced-order model of the near-wall flow. Following this, The University of Queensland's Eilmer CFD solver [5] will be used to replicate expansion tube experiments of recent ice giant heat flux experiments to determine how the predicted surface heat flux varies across different species diffusion models and catalytic wall boundary conditions when applied to a realistic test model geometry.

REFERENCES

[1] M. Hofstadter, A. Simon, S. Atreya, D. Banfield, J. J. Fortney, A. Hayes, M. Hedman, G. Hospodarsky, K. Mandt, A. Masters, M. Showalter, K. M. Soderlund, D. Turrini, E. Turtle, K. Reh, J. Elliott, N. Arora, A. Petropoulos, *Planetary and Space Science* **177**11 (2019), 10.1016/j.pss.2019.06.004.

[2] G. Palmer, D. Prabhu, B. A. Cruden, *Journal of Spacecraft and Rockets* (American Institute of Aeronautics and Astronautics Inc., 2014), 801–814.

[3] J. A. Rataczak, I. D. Boyd, J. W. McMahon, *Journal of Thermophysics and Heat Transfer* 1–226 (2025).

[4] L. LEES, *Journal of Jet Propulsion* **26**, 259–2694 (1956).

[5] N. N. Gibbons, K. A. Damm, P. A. Jacobs, R. J. Gollan, 6 (2022), 10.1016/j.cpc.2022.108551.

A neural network based non-equilibrium reaction model for DSMC

S. Trivedi[1,a)], K. S. Jung[2], A. W. Jasper[3], J. K. Harvey,[4] and J. H. Chen[1]

[1]*Sandia National Laboratories, Livermore, CA, USA.*
[2]*Pukyong National University, Busan, South Korea.*
[3]*Argonne National Laboratories, Lemont, IL, USA.*
[4]*Department of Engineering, University of Cambridge, Cambirdge, UK.*

[a)]Corresponding author: strived@sandia.gov

State-specific reaction rates were implemented in the DSMC code SPARTA [1] using a neural-network (NN)–based approach. The state-specific reaction rates were obtained from quasi-classical trajectory (QCT) calculations for reactions in the hydrogen–air mechanism.

A single-hidden-layer NN with a hyperbolic tangent activation function was used,

$$y = W_2 \tanh(W_1 x + B_1) + B_2, \tag{1}$$

where y is the reaction rate and $x = [T,\ E_{\text{vib}}]^T$ is the input vector. The weight matrices and bias vectors are $W_1 \in \mathbb{R}^{N\times 2}$, $W_2 \in \mathbb{R}^{1\times N}$, $B_1 \in \mathbb{R}^{N\times 1}$, and $B_2 \in \mathbb{R}$, where N is the number of hidden nodes. This compact representation allows both fine and coarse QCT datasets to be used, while the total number of model parameters depends only on N.

As an initial step, the NN model was trained independently of the DSMC implementation to obtain the model coefficients. The chain-branching reaction $H + O_2 \rightarrow OH + O$ was used to assess the approach. Reaction rates from the QCT calculations were generated over a range of T, with several E_{vib} values corresponding to each temperature. These data were used as inputs to the NN model. Eighty percent of the dataset was used for training and the remainder for testing. The results are shown in Fig. 1.

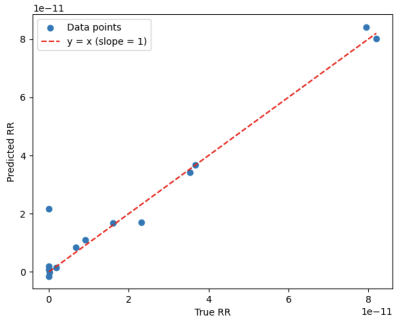


Fig. 1. True reaction rate versus the NN-predicted reaction rate. The red dashed line represents $y = x$, and the blue symbols denote the predictions. The agreement is close over most of the range, with noticeable deviation only at very low reaction-rate values.

The resulting NN coefficients will be subsequently implemented in DSMC to predict reaction rates over an extended range of thermochemical conditions. These will then be used to simulate 1-D and 2-D hydrogen–air detonations with strong vibrational non-equilibrium.

ACKNOWLEDGEMENTS

The work is supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA- 0 0 03525. The computational resources were provided by National Energy Research Scientific Computing Center (NERSC) and Oak Ridge Leadership Computing Facility (OLCF).

REFERENCES

[1] S. J. Plimpton, M. A. Gallis, Sparta, http://sparta.sandia.gov, .

Zeeman spectroscopy of hypersonic flow in a magnetic field

T. J. McIntyre,[1,a)], D. E. Gildfind,[2], Y. Liu,[2], N. Temme,[2], C. Yu,[2] and S. G. Lock[2]

[1]*The University of Queensland, School of Mathematics and Physics, Brisbane, 4072, Australia.*
[2]*The University of Queensland, School of Mechanical and Mining Engineering, Brisbane, 4072, Australia.*

[a)]Corresponding author: t.mcintyre@uq.edu.au

Magnetohydrodynamic braking has been proposed as a potential alternative to conventional drag for decelerating a space vehicle as it enters a planetary atmosphere. In this approach, a strong magnet is placed within the vehicle creating a magnetic field that interacts with charged particles in the surrounding flow. The resulting Lorentz force on the electrons in the flow leads to a reaction force opposing the motion of the vehicle. However, this interaction is complex, and there are ongoing studies to understand the flow physics and to optimise performance [1].

One approach for studying the flow physics is to use emission spectroscopy to examine excited state populations of atomic species in the flow. The presence of an applied (and then induced) magnetic field leads to the Zeeman effect where degenerate energy levels are split into separate levels and the resulting spectra can be analysed to infer the strength of the magnetic field. Furthermore, Stark broadening can be used to measure the local electron number density and this, together with the measured magnetic field can be compared to numerical modelling of the flow.

Experimental measurements were conducted in the X2 expansion tube at the University of Queensland. An argon test gas with a free-stream speed of around 6 km/s and a density of 0.001 kg·m^{-3} was used ensuring appropriate levels of ionisation in the flow, and accessible optical transitions. A spherical test model with a diameter of 38 mm was placed in the flow either in the form of a steel ball or a permanent 0.8 T magnet. Fig. 1 shows the experimental arrangement and sample spectra for the steel ball (upper) and magnet (lower), along with modelled spectra. The flow over the magnet shows Zeeman splitting allowing for an estimate to be made of the magnetic field at this location. A full set of measurements and associated analysis will be presented at the conference.

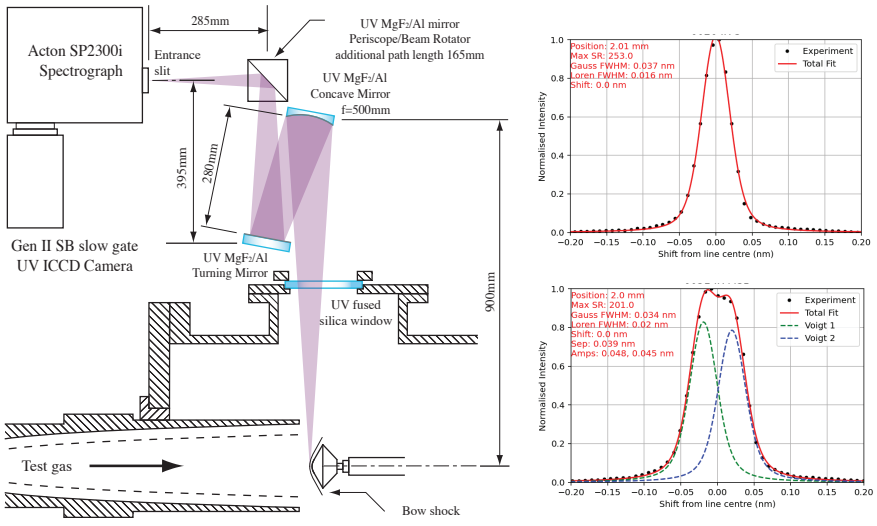


Fig. 1. Experimental arrangement and sample spectra.

ACKNOWLEDGEMENTS

This research was supported by the Australian Government through the Australian Research Council's Discovery Projects funding scheme (DP220101478). C. Yu and S.G. Lock are both recipients of the Research Training Program Scholarship of UQ. The authors wish to thank Mr Neil Duncan for technical support, and X2 operators for their assistance in conducting experiments.

REFERENCES

[1] A. Lefevre, D. E. Gildfind, R. J. Gollan, P. A. Jacobs, C. M. James, *AIAA Journal* **60**, 5046–5059 (2022).

Abstract 177

Optimisation of X2 Schlieren System for Studying Nonequilibrium Low Density Hypersonic Flows

S. Goetjens[1], S. G. Lock[1], R. G. Morgan[1] and C. M. James[1]

[1] *Centre for Hypersonics, School of Mechanical and Mining Engineering, The University of Queensland, St Lucia, QLD, 4072, Australia*

[a)] Corresponding author: s.goetjens@uq.edu.au

Nonequilibrium chemistry occurs due to the high temperature post shock where there is a lack of sufficient time for the molecules and atoms to reach chemical or thermal equilibrium and they occur over appreciable length scales. Post-shock nonequilibrium chemistry will influence the performance of hypersonic vehicles in low density environments such as at high altitudes. These performance effects include the heat transfer, the forces, and vehicle flight controls. Changes in the chemistry post-shock of a vehicle can be used to track the vehicle. Computational Fluid Dynamics codes with a finite-rate chemistry model were developed to model this behaviour but there were many uncertainties related to the quality of reaction rates themselves. The standard air chemistry models developed by [1] and [2], were roughly curve fits to data from 1960s to 1970s. A new method called the Modified Marrone-Treanor thermochemical nonequilibrium air chemistry model, proposes to change the understanding of post-shock nonequilibrium chemistry for hypersonic vehicles.

To capture high-quality data for this phenomenon, a Schlieren system will be used, specifically, it will be used to measure the shock standoff distance which is the seperation between the front of a detached shock wave and the surface of an blunt object in hypersonic flow. A Schlieren system provides an accurate, non-destructive and very sensitive method to capture hypersonic flow. Schlieren imaging uses the differing refractive indices of different substances of varying velocities when passed through the system. The traditional Z-fold Schlieren geometry has several issues such as of-axis aberration, particularly coma and astigmatism [3]. Equal and opposite off-axis angles on the collimator and focusing mirrors can eliminate coma while large f-number mirrors (larger than f/8) can minimise astigmatism [3]. However, large f-number mirrors can have a large system footprint so to minimise the system's footprint, off-axis parabolic mirrors can be used which permit smaller f-number mirrors without increasing the system's footprint [3].

A large Schlieren system replicated [3]'s design using off-axis parabolic mirrors for X2 and preliminary testing was conducted [4]. An optimisation attempt created a 29% smaller system footprint [5] but still had spatial limits for the testing of instruments within the test section. To better use this empty space, the Schlieren system was further miniaturised to allow other instruments to be used within the vicinity of the Schlieren system. To reduce the system size, lenses was used to shorten the focal lengths of mirrors, reduce errors in Schlieren windowing issues and provides flexibility to achieve different fields of views for different experiments. Optimisation will add additional parameters to reduce any distortion and inefficiency effects.

In addition, manual optomechanical mounts will improve the need for adjustment of the system, if needed and will make alignment of the system much easier. The laboratory of the X2 Super-Orbital Expansion Tube is located in a high people traffic area so accidental bumps to the Schlieren system may occur. Future improvements for the Schlieren system will include motorised mounts instead of manual mounts to allow improved control of the mirrors. A Class 4 laser will be used because it can emit more power than a LED source. For safety precautions, a cover for the entire Schlieren system, a curtain surrounding the Schlieren system was implemented and an emergency stop button.

REFERENCES

[1] Gupta, RN, Yos, JM, Thompson, RA & Lee, K. *A Review of Reaction Rates and Thermodynamic and Transport Properties for an 11-Species Air Model for Chemical and Thermal Nonequilibrium Calculations to 30,000 K* NASA Reference Publication 1232 (NASA, 1990).

[2] Park, C. Review of chemical-kinetic problems of future NASA missions. I – Earth entries. *Journal of Thermophysics and Heat Transfer* **7,** 385-398. ISSN: 1533-6808 (July 1993).

[3] Zheng, L., Susa, A. J., & Hanson. R. K. (2022). *Methodology of designing compact schlieren systems using off-axis parabolic mirrors*. *61*(16), 4857-4864. https://doi.org/10.1364/AO.457151

[4] Bui, T. (2023). *Testing of a Free-Flying Hypersonic Gilder in an Expansion Tube* [Undergraduate thesis, University of Queensland]. UQ eSpace. https://espace.library.uq.edu.au/data/UQ_3d7b8ad/Thien_Bui_Thesis.pdf

[5] Slennett-Roberts, J. *Commissioning of an Off-Axis Parabolic Schlieren System for Hypersonic Flow Visualisation in UQ's X2 Expansion Tube.* [Undergraduate thesis, University of Queensland]. UQ eSpace. https://doi.org/10.14264/1b2841d

Abstract 178

Plume Impingement Software Module for Real-Time Proximity Operations

K. J. Higdon[1,a)] and W. H. Yu[2]

[1]*Rarefied Studios, LLC, 4500 Vista Dr., Fort Collins, CO 80526, USA*
[2]*NASA Goddard Space Flight Center, 8800 Greenbelt Road, Greenbelt, MD 20771, USA*

[a)] Corresponding author: kyle.higdon@rarefiedstudios.com

Successfully executing proximity operations in space, such as docking or in-orbit servicing, requires sophisticated spacecraft design that accounts for induced environments. As a chaser vehicle's attitude control thrusters fire, they create rarefied plumes that can impact the target vehicle, with the potential to overload components, exceed thermal limits, and spin the target vehicle out of control. High-fidelity simulations of the thruster plume impingement environment require the direct simulation Monte Carlo (DSMC) method, but DSMC is too computationally expensive to simulate proximity operations that involve thousands of thruster firings. For this analysis to be tractable, engineering models of the plume flowfield and impingement events are used to simulate these trajectories [1]. Currently, on-orbit plume impingement environments are modeled through an inefficient open-loop analysis cycle where the vehicle's flight controller and plume impingement teams iterate on the trajectories until they pass the target vehicle's plume requirements.

As complex on-orbit missions evolve and become more frequent, lengthy design cycles will become operational bottlenecks. To address this gap, this work develops an advanced plume impingement module capable of operating at real-time scale that can be integrated with existing mission planning tools and onboard flight systems. The plume module leverages state-of-the-art plume simulation techniques [2] to deliver fast, physics-based impingement predictions in a software architecture that can be tailored to diverse proximity operations scenarios. A prototype of this plume impingement module is built to demonstrate the feasibility of real-time performance. This prototype completes plume impingement calculations in microseconds per target geometry mesh point. The software serves as a foundational capability for plume-aware trajectory design, operational risk assessment, and future autonomous decision-making systems.

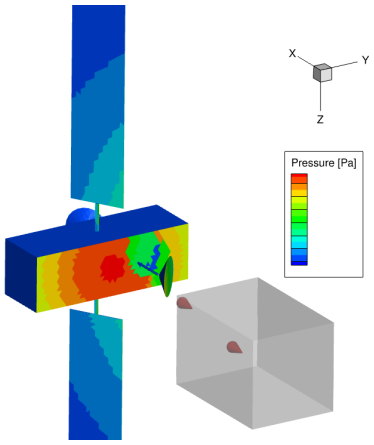


Fig. 1. Plume Impingement Pressure for a Demo Dual-Jet Firing.

ACKNOWLEDGEMENTS

This work was supported by a NASA Small Business Innovation Research Grant (#80NSSC25C0327).

REFERENCES

[1] K. J. Higdon, F. E. Lumpkin, "On-Orbit Plume Impingement Overview," NASA NTRS 20240013965, 2025.
[2] G. A. Simons, "Effect of nozzle boundary layers on rocket exhaust plumes." *AIAA Journal*, Vol. 10, No. 11, 1972.

Abstract 179

Dimension-reduced Simulation of Hypersonic Vibrational Non-Equilibrium Flows Using DSMC Method

Zi-Xin Liu[1] and Zhi-Hui Wang[1,2 a)]

[1]*School of Engineering Science, University of Chinese Academy of Sciences,101408, Beijing, PR China*
[2]*State Key Laboratory of Nonlinear Mechanics, Chinese Academy of Sciences, 100190, Beijing, PR China*

[a)] Corresponding author: wisdom@ucas.ac.cn

The rapid and accurate prediction of aerodynamic heating remains a great challenge in designing new-generation near-space hypersonic vehicles, especially when the non-equilibrium real gas effects are significant. These vehicles typically operate in regimes characterized by combined strong shear and compression, along with significant influences from vibrational excitation at altitudes of 30-50 km. However, it requires prohibitively large computational resources to perform full-scale numerical simulation for hypersonic vehicles under high Mach number and moderate-to-low Reynolds number conditions. Consequently, it is generally necessary to adopt reasonable simplifications or dimensionality reduction based on physical analysis.

The most classic theory regarding hypersonic flow similarity is the hypersonic equivalence principle[1], based on the inviscid assumption and small perturbation theory. It establishes the equivalence between steady inviscid flow and dimension-reduced unsteady flow, providing a simplified computational method. On this basis, the generalized hypersonic equivalence principle(GHEP) based on physical similarity was proposed by Wang et al.[2,3,4], taking the effects of viscosity into account and demonstrating the dimension-reduced unsteady model can accurately reproduce the surface heat flux of the steady hypersonic viscosity flow under the calorically perfect gas assumption. However, in the high-temperature flow fields surrounding a hypersonic vehicle, the vibration excitation effects could play a significant role[5]. This paper investigates the aeroheating similarity between a steady viscosity flow and a corresponding dimension-reduced unsteady flow dominated by vibrational excitation effects, as an extension of the GHEP. The direct simulation Monte Carlo (DSMC) method is employed to investigate hypersonic near-continuum flows over a flat plate, covering regimes from shear-dominated flow to combined shear-compression-dominated flow at an angle of attack. Firstly, for the shear-dominated flow, where characteristic timescale of the flow is relatively very short, which means the vibrational energy freezes, the impact of vibrational energy incomplete accommodation on this equivalence principle is investigated. Secondly, for combined shear and compression-dominated flow, where the characteristic timescale of the flow is comparable to the vibrational relaxation timescale, the influence of vibrational non-equilibrium on this equivalence principle is studied. Quantitative comparisons indicate that, the surface heat flux in the steady non-equilibrium flow can be accurately reproduced by the dimension-reduced unsteady model, validating the applicability of GHEP in the high-temperature real gas flow regime.

This work further extends the generalized hypersonic equivalence principle to more realistic real gas flows accounting for vibrational excitation, significantly reducing the time and computational resources required for numerical simulations, and showing a potential significance for the engineering practice.

ACKNOWLEDGEMENTS

This work was supported by the Strategic Priority Research Program (B) of Chinese Academy of Sciences (grant XDB0620203).

REFERENCES

[1] J. D. Anderson, Hypersonic and High-temperature Gas Dynamics, 3rd ed. (2019).
[2] Z.-H. Wang, AIAA Journal, **58**, 255-264 (2020).
[3] Z.-H. Wang, AIP Conference Proceedings 2132, 070022 (2019).
[4] H.-J. Gao, Z.-H. Wang, AIP Conference Proceedings 2996, 140006 (2024).
[5] Nompelis I, Candler G V, Holden M S, AIAA Journal, **41**, 2162-2169(2003).

A Quasi-1D Stagnation Line Solver for designing Hypersonic Non-Equilibrium Experiments

T J. Rossini[1,a)], T J. van den Herik[1] and C M. James,[1]

[1]*Centre for Hypersonics, School of Mechanical and Mining Engineering, The University of Queensland, St Lucia, QLD 4072, Australia.*

[a)]Corresponding author: t.rossini@uq.edu.au

Due to the associated limitations of ground based facilities, the free stream flow can never be exactly recreated, and very rarely will the full-scale model be of such a size that it can fit within the facility core flow. Thus, the hypersonic similitude laws must be applied. For blunt body experiments generally binary scaling is used, where $(\rho_\infty L)_{flight} = (\rho_\infty L)_{laboratory}$, reproducing binary (two-body) reactions such as dissociation and ionisation [1]. Binary scaling also requires that the total enthalpy ($H_t \approx \frac{1}{2} \cdot u_\infty^2$) is conserved between the free stream and ground tests as this provides the energy required for chemistry to occur. This approximately matches the chemical length scales and non-equilibrium region governed by the gas Damköhler number (Da_g) [2]. However, since chemical equilibrium (due to recombination) is a weak function of pressure, often matching the free stream Da_g does not exactly recreate the post shock conditions. Thus, perfectly recreating post shock conditions in a ground based facility is difficult, previously, analysis and verification of the flow conditions was either done using equilibrium chemistry estimations using NASA's Chemical Equilibrium with Applications (CEA) or non-equilibrium calculations using GDTK's simple post-normal-shock relaxation (POSHAX), which ignores the large effect that geometry has on the post-shock relaxation. However, both tools do not give the full picture, and running a fully resolved 2D simulation is not always computationally or practicality viable as often the goal is to run on the order of hundreds of simulations to determine target conditions.

This prompted the development of a quasi-1D non-equilibrium stagnation line solver (NESL), allowing accurate predictions of shock standoff, stagnation point heating and the study of non-equilibrium chemical relaxation, all without the computational cost of a 2D simulation. A technique will be presented, differing from the classical use of the Dynamically Reduced Navier-Stokes Equations (DRNSE) developed by Klomfass and Müller [3] for quasi-1D flow. Discretisation of the governing equations using the Finite Volume Method (FVM) allows for inherent shock-capturing and does not require shock-fitting using the rankine-hugoniot jump conditions and/or empirical correlations for shock-standoff or curvature like other implementations [4–7]. The proposed method is derived from the full 2D Navier-Stokes Equation in Cartesian coordinates, where the system of equations is simplified using the assumption that that there is no vertical velocity ($v = 0$) along the stagnation line, and closed with Newtonian theory to describe the pressure distribution around the body. However, these assumptions do impose limits on the conditions that can be simulated, such that only hemispherical bodies (cylinders and spheres) and flows where the thin shock layer assumption is valid ($\approx M > 5$) can be tested, which covers a large envelope of what is tested in expansion tube facilities.

Preliminary testing using the validation case conducted in the HEG shock tunnel at the German Aerospace Center (DLR) [8] showed great agreement between experimental measurements, higher dimension numerics and NESL simulations. The results have been summarised in Tab. 1. Note, descripencies in heat flux are due to the lack of catalytic wall boundaries which will soon be implemented.

Tab. 1. Comparison of Experimental, NESL, 2D and 3D Results from HEG run 627 [8].

Method	Shock Standoff (mm)	Heat Flux (MW/m^2)	Stagnation Pressure (kPa)
NESL	11.33	4.24	69.83
Experimental	12.15	4.82	68.52
2D Numerical	12.60	4.80	71.00
3D Numerical	11.70	4.80	71.00

REFERENCES

[1] C. M. James, *Designing Expansion Tube Conditions* 24–30 (2025).
[2] O. Chazot, *Ground Testing Strategy for High-Speed Re-entry* 3–8 (2026).
[3] A. Klomfass, S. Müller, *Shock Waves* **7**, 13–23 (1997).
[4] C.-H. Lee, *International Journal of Aeronautical and Space Sciences* **17**, 149–156 (2016).
[5] Q. Hong, X. Wang, Y. Hu, Q. Sun, *Physics of Fluids* **32** (2020), 10.1063/5.0003247.
[6] C. Song, S. Quanhua, *Chinese Journal of Aeronautics* **29**, 1517–1526 (2016).
[7] T. B. Petrova, G. M. Petrov, J. R. Maxwell, J. R. Peñano, *Physics of Plasmas* **32** (2025), 10.1063/5.0261029.
[8] K. Hannemann, *41st Aerospace Sciences Meeting and Exhibit*, January (2003), 10.2514/6.2003-978, aIAA Paper 2003-0978.

Maximising Vibrational Nonequilibrium in Supersonic Nozzle Flows

D. J. Petty[1,a)]

[1]*School of Engineering and Technology, University of New South Wales Canberra, Campbell, ACT, Australia*

[a)]Corresponding author: d.petty@unsw.edu.au

Rapid expansion of highly energised molecular gases through a converging-diverging nozzle can result in a large degree of vibrational nonequilibrium. Under such conditions, stimulated emission can occur in a process known as gasdynamic lasing. The power and efficiency of a gasdynamic laser is directly related to the degree of vibrational nonequilibrium achieved during expansion. Quasi one-dimensional supersonic nozzle calculations are used to predict the vibrational nonequilibrium of carbon monoxide and carbon dioxide in mixtures of helium, oxygen and nitrogen using a state-to-state kinetics model [1, 2]. Enforcing the sonic choke condition is achieved via unconstrained optimisation of a nonlinear transform applied the quasi-1D equations, which improves the speed and robustness of the nozzle calculations. The solver incorporates automatic differentiation which provides gradients [3] of the exiting vibrational populations with respect to all the parameters that define the reservoir gas mixture conditions and nozzle geometry. Sensitivity of the vibrational populations to various input parameters will be presented, as well as the optimal gaseous mixture and nozzle configuration which maximises the aggregate deviation of vibrational populations relative to the Boltzmann distribution.

REFERENCES

[1] C. Fromentin, T. Silva, T. C. Dias, A. S. Morillo-Candas, O. Biondo, O. Guaitella, V. Guerra, *Plasma Sources Science and Technology* **32**, 024001 (2023).
[2] C. Fromentin, T. Silva, T. C. Dias, E. Baratte, O. Guaitella, V. Guerra, *Plasma Sources Science and Technology* **32**, 054004 (2023).
[3] D. J. Petty, S. O'Byrne, *AIP Conference Proceedings* (AIP Publishing LLC, 2024) 060009.

Abstract 184

Two-Dimensional Hybrid PIC Simulation of Hall Thrusters with Artificial Magnetic Field Disturbances

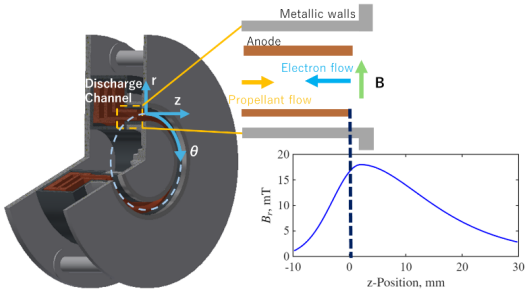
Hayate Osawa[1,a)], Takuto Ogawa[1], Akira Furuya[1], Shunsuke Amikura[1], and Rei Kawashima[1]

[1] *Department of Electrical Engineering and Computer Science, Shibaura Institute of Technology, Tokyo, Japan*

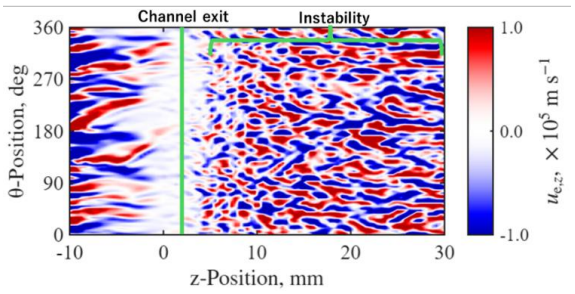
[a)] Corresponding author: AE21028@shibaura-it.ac.jp

Hall thrusters for electric propulsion generate thrust by generating rarefied plasma with magnetic field confinement of electrons. For efficient plasma generation, the magnetic field distribution is designed to have its peak around the channel exit, as shown in Fig. 1(left). The electron flow confined by the magnetic field in Hall thruster is affected by anomalous electron transport. In this phenomenon, electrons flow more across the magnetic field lines than theoretically predicted. The experiment showed that electron transport is significantly enhanced in the plume region. [1] Recent numerical simulations on rarefied plasma revealed that the anomalous electron transport in plume region is affected by azimuthal instabilities, such as gradient drift instability shown in Fig. 1(right). The relation between the azimuthal plasma properties and electron transport in Hall thrusters has also been investigated in experiments. Bak et al. enhanced electron transport in Hall thrusters with non-uniform propellant supply in the azimuth direction. [2] An azimuthal non-uniform supply of propellant increases the discharge current over the entire discharge region. An increase in discharge current was also observed in Hall thrusters with non-axisymmetric magnetic field. [3]

This study aims an active control of anomalous electron transport by using artificial magnetic disturbances. In this study, propellant is supplied uniformly along the azimuthal direction of the Hall thruster, and the magnetic field is artificially disturbed either in the θ direction or over time (t direction). We performed two-dimensional hybrid Particle-in-Cell (ion particles and electron fluid) simulations in the Z-θ direction, to investigate the plasma characteristics of Hall thrusters with non-uniform magnetic fields. We discuss the effects of the artificially disturbed magnetic fields on the electron transport enhancement or reduction.



(Left). Structural of an anode layer Hall thruster and z-direction magnetic field distribution in the hall thruster discharge channel



(Right). Azimuthal instability of electrons (z- θ)

Fig. 1. Hall thruster overview (left) z-direction electron velocity (right)

ACKNOWLEDGEMENTS

This work was supported by JSPS KAKENHI Grant Numbers JP24K01084.

REFERENCES

[1] Koo, J. W. and Boyd, I. D.: Modeling of anomalous electron mobility in Hall thrusters, Physics of Plasmas, 13 (2006) pp. 033501–7

[2] Bak, J., Van Loo, B., Kawashima, R. and Komurasaki, K.: Discharge characteristics and increased electron current during azimuthally nonuniform propellant supply in an anode layer Hall thruster, J. Appl. Phys., 128 (2020), 023302

[3] J. Bak, R. Kawashima, G. Romanelli, and K. Komurasaki: Plasma structure and electron cross field transport induced by azimuthal manipulation of the radial magnetic field in a Hall thruster E × B discharge, J. Appl. Phys. 131, 053302 (2022)

Velocity Distribution of Water Molecules Evaporating From a Liquid Surface: Molecular Beam Experiment and Molecular Dynamics Simulation

I. Kinefuchi[1,a)], K. Sato[2], and A. Fujita[2]

[1] *Department of Human and Engineered Environmental Studies, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa-shi, Chiba 277-8563, Japan*
[2] *Department of Mechanical Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*

[a)] Corresponding author: kine@fel.t.u-tokyo.ac.jp

The analysis of gas–liquid two-phase flows with phase change requires boundary conditions at liquid–vapor interfaces that give the mass flux and temperature jump due to evaporation and condensation [1]. A strongly nonequilibrium gas flow region, known as the Knudsen layer, forms in the vicinity of a liquid surface where a net evaporation or condensation flux exists. The boundary conditions for the mass, momentum, and energy fluxes at a gas–liquid interface can be derived by solving nonequilibrium gas flows within the Knudsen layer. However, most analyses conducted so far have assumed that molecules evaporating from a liquid surface follow the Maxwell–Boltzmann distribution, even under nonequilibrium conditions with a net evaporation or condensation flux. Ishiyama et al. [2] demonstrated, using molecular dynamics simulations, that the velocity distribution of evaporating molecules deviates from the half-Maxwellian distribution. Nevertheless, no experimental study has directly measured the velocity distribution of evaporating molecules. Furthermore, establishing accurate interfacial boundary conditions for macroscopic fluid analyses requires a more detailed characterization of the velocity distribution function of evaporating molecules.

In this study, we experimentally measured the velocity distribution of water molecules evaporating from a liquid surface using the molecular beam technique [3]. By employing a nanoporous array membrane to sustain a liquid surface under vacuum conditions, we realized a free-molecular condition that suppressed intermolecular collisions among evaporated molecules, enabling direct measurement of the intrinsic velocity distribution immediately after evaporation. The measured distribution shows a lower population of low-velocity molecules than the half-Maxwellian distribution. This tendency is consistent with the results of the molecular dynamics simulations. The velocity distribution obtained from the molecular beam experiment can be reproduced by a velocity distribution function that incorporates the attractive potential near the liquid surface. The potential depth determined to reproduce the experimental results is in reasonable agreement with the value estimated from the vapor-to-liquid density ratio under the vapor–liquid equilibrium condition. We also conducted molecular dynamics simulations and found that, in water systems, the method used to evaluate long-range interactions markedly alters the resulting velocity distribution.

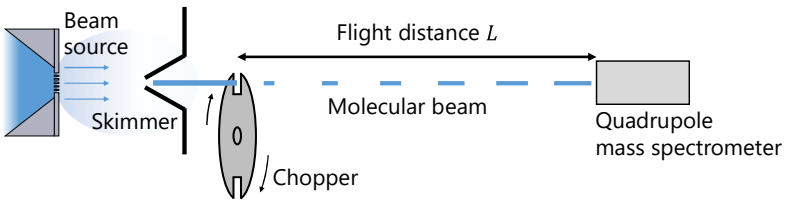


Fig. 1. Schematic of the molecular beam measurement of evaporating molecules from a liquid surface

ACKNOWLEDGEMENTS

This work was supported by JSPS KAKENHI Grant Numbers JP23K26033 and JP25K21678.

REFERENCES

[1] E. Aursand, T. Ytrehus, *International Journal of Multiphase Flow,* **116**, pp. 67–79 (2019).
[2] T. Ishiyama, T. Yano, S. Fujikawa, *Physics of Fluids*, **16**, pp. 4713–4726 (2004).
[3] G. Scoles (ed.), *Atomic and Molecular Beam Methods: Vol. 1* (Oxford University Press, New York, 1988).

Realistic Gas-surface Interaction (GSI) model for Atmosphere-Breathing Electric Propulsion (ABEP) Intake Design

A. Appar[1,a)] and S. J. Poovathingal[2]

[1]*Department of Aerospace Engineering, Universidad Carlos III de Madrid, Leganés, 28911, Madrid, Spain.*
[2]*Department of Mechanical and Aerospace Engineering, University of Kentucky, Lexington, 40506, KY, USA.*

[a)]Corresponding author: ahilan.appar@uc3m.es

The performance and mission viability of very low Earth orbit (VLEO) spacecraft depend sensitively on accurate predictions of aerodynamic drag and intake collection efficiency in the rarefied, hyperthermal atomic oxygen (AO) environment. Building on our previously developed diffuse–Cercignani–Lampis–Lord (DCLL) gas–surface interaction (GSI) model for AO–silica system [1], we extend the molecular dynamics (MD) database to cover a full range of incidence angles (5°–90°) and extract angle-dependent DCLL accommodation parameters for use in the widely-used open-source particle solver SPARTA, based on the direct simulation Monte Carlo (DSMC) approach. Using this angle-resolved DCLL model, we perform system-scale simulations of canonical VLEO configurations, including simple plates and cylinders, to quantify realistic drag coefficients and compare them with conventional diffuse/specular reflection assumptions. We then analyse atmosphere-breathing electric propulsion (ABEP) intake and gas-concentrator concepts, evaluating how accurately GSI modelling predicts mass flow capture, compression ratios, and overall collection efficiency relative to standard engineering models. The results highlight regimes where detailed GSI physics has a first-order impact on drag, intake performance, and thus on orbit maintenance and power requirements for VLEO platforms. This work demonstrates how a molecularly informed, yet computationally tractable DCLL model can be propagated up to the system level, providing more reliable aerodynamic and performance predictions for the design of next-generation VLEO satellites and ABEP systems.

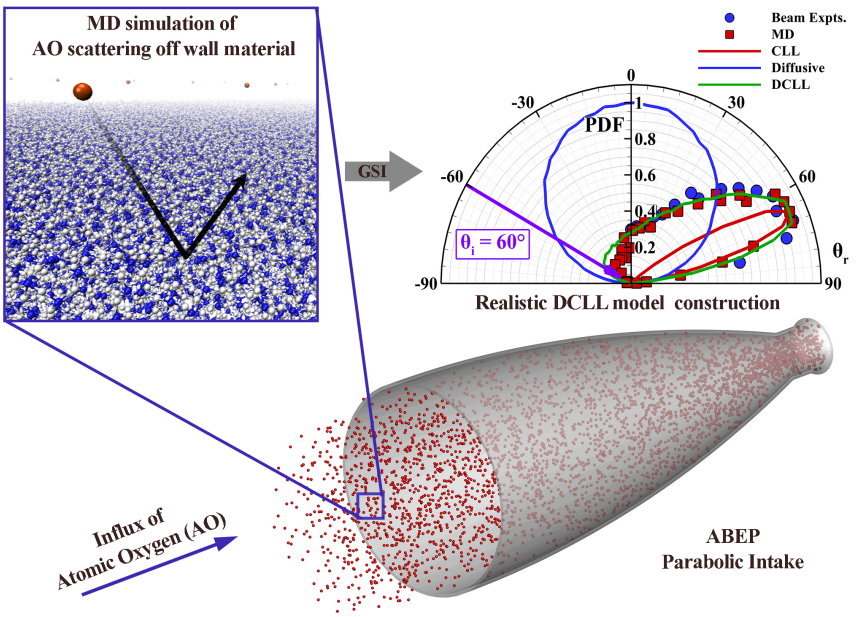


Fig. 1. Schematic representation of realistic gas-surface interactions on ABEP intake wall material.

ACKNOWLEDGEMENTS

This work was supported in part by the UC3M Young Doctor Award 2025/00863/001 (Appar) and the DARPA Young Faculty Award D24AP00309 (Poovathingal), with contributions from both institutions.

REFERENCES

[1] A. Appar, S. J. Poovathingal, *Aerospace Science and Technology,* 111550 (2025).

Weakly Nonlinear Drag Induced by Uniform Surface Heating of a Sphere

S. Taguchi[1,a)], K. Ko,[1] and T. Tsuji[1]

[1] *Graduate School of Informatics, Kyoto University, Kyoto, Japan.*

[a)] Corresponding author: taguchi.satoshi.5a@kyoto-u.ac.jp

The sphere drag in the slow-flow regime is a classical problem in rarefied gas dynamics. In addition to the drag, under rarefied conditions, the flow induced by a nonuniform surface temperature and the resulting force, referred to as thermophoresis, have been extensively studied [1, 2]. In a different scenario, a particle may be uniformly heated and move through a gas. In this case, any modification of the drag arises only beyond the linear approximation, since the induced temperature field remains isotropic at linear order. The nonlinear coupling between the external flow and the surface heating then generates an asymmetry in the flow field, leading to a nontrivial correction to the drag. Such a nonlinear mechanism was examined in the near-continuum regime for large temperature differences [3]. Here we consider the complementary regime in which the temperature difference is small while the Knudsen number is $O(1)$, i.e. the transitional regime. The problem serves as a minimal kinetic model for a laser-heated Au nanoparticle immersed in a gas, where the molecular mean free path is comparable to the particle diameter.

We consider a fixed sphere of radius L placed at the origin of a Cartesian coordinate system X_i, $i = 1, 2, 3$. Far from the sphere, the gas is in a uniform equilibrium state with density ρ_0, velocity $\boldsymbol{v}_0 = (v_0, 0, 0)$, and temperature T_0, so that the pressure is $p_0 = \rho_0 R T_0$, where R is the specific gas constant. The sphere surface is maintained at a uniform temperature $T_w \neq T_0$. No external force is applied. The steady flow of the rarefied gas around the heated sphere is described by the Boltzmann equation with the Maxwell boundary condition at the surface. The Knudsen number is defined by $\mathrm{Kn} = \ell_0/L$, where ℓ_0 is the molecular mean free path evaluated at the reference state. The Reynolds number is defined by $\mathrm{Re} = \rho_0 L v_0/\eta_0$, where $\eta_0 = \eta(T_0)$ is the gas viscosity at temperature T_0.

When $T_w = T_0$, the drag force reduces to the classical Stokes value $\boldsymbol{F}_D = 6\pi\eta_0 L\boldsymbol{v}_0$ in the limits $\mathrm{Re} \to 0$ and $\mathrm{Kn} \to 0$. Our objective is to determine how this drag is modified when $T_w \neq T_0$, assuming $\mathrm{Re} \ll 1$ and $\mathrm{Kn} = O(1)$.

We perform an asymptotic analysis of the Boltzmann system using the small parameter $\epsilon = v_0/\sqrt{2RT_0}$, assuming a weakly nonlinear regime in which $|T_w - T_0|/T_0 = O(\epsilon)$. Under this scaling, inertial and thermal effects enter at the same asymptotic order. The solution is constructed using a matched asymptotic expansion [4]. As a result, we obtain the drag force in the form

$$\boldsymbol{F}_D = 6\pi\eta_0 L\boldsymbol{v}_0\left[\left(1 + \frac{3}{8}\bar{h}_D\mathrm{Re}\right)\bar{h}_D + \frac{5}{12}\frac{T_w - T_0}{T_0}\left(\frac{3}{10} + T_0\left(\frac{d\ln\eta}{dT}\right)_0\right)\bar{h}_D^T\right], \quad \mathrm{Re} \ll 1,$$

where $(d\ln\eta/dT)_0 = \eta_0^{-1}(d\eta(T)/dT)_{T=T_0}$ and $\bar{h}_D$ and $\bar{h}_D^T$ are correction functions depending on the Knudsen number and the accommodation coefficient of the surface. Both functions approach unity in the continuum limit $\mathrm{Kn} \to 0$. These correction functions are evaluated numerically based on the Bhatnagar–Gross–Krook (BGK) model. The present analysis also extends the work of Kassoy et al. [5], who studied a related problem within the compressible Navier–Stokes framework, by incorporating kinetic effects at finite Knudsen numbers. The analysis elucidates the asymptotic structure of the nonlinear drag induced by uniform surface heating at finite Knudsen numbers.

ACKNOWLEDGEMENTS

This work was supported by JSPS KAKENHI Grant Numbers JP24K00803 and JP25K01156.

REFERENCES

[1] S. Takata, Y. Sone, *Eur J. Mech. B/Fluids* **14**, 487–518 (1995).
[2] D. Kalempa, F. Sharipov, *J. Fluid Mech.* **900**, A37 (2020).
[3] V. S. Galkin, M. N. Kogan, O. G. Fridlender, *PMM-J Appl. Math. Mec.* **36**, 829 – 833 (1972).
[4] S. Taguchi, *J. Fluid Mech.* **774**, 363–394 (2015).
[5] D. R. Kassoy, T. C. Adamson, A. F. Messiter, *Phys. Fluids* **9**, 671–681 (1966).

Raman mapping of gas flow field inside a submillimeter channel

José M. Fernández[1] and **Guzmán Tejeda**[1,a)]

[1] *Laboratory of Molecular Fluid Dynamics, Instituto de Estructura de la Materia IEM-CSIC, Madrid, Spain*

[a)] Corresponding author: *g.tejeda@csic.es*

High sensitivity Raman spectroscopy, has demonstrated to be a non intrusive and powerful diagnostics technique for molecular gas flows: density and rotational temperature can be measured at different points of the flow field [1, 2] with high spatial resolution (a few microns). Recently we have extended Raman diagnostics to work inside confined flows in millimeter channels [3].

In this work we present a experimental study of the gas flow along transition from a reservoir to a expansion chamber through a submillimeter glass channel. By combining the free jet diagnostic technique and the confined flow one, we have developed a new experimental setup and methodology that allows to probe temperature and density of the flowing gas (pure N_2, air and H_2) by means of Raman spectroscopy at the entrance, inside and exit of the glass channel. Some example of Raman spectra obtained in this work are shown in Fig. 1.

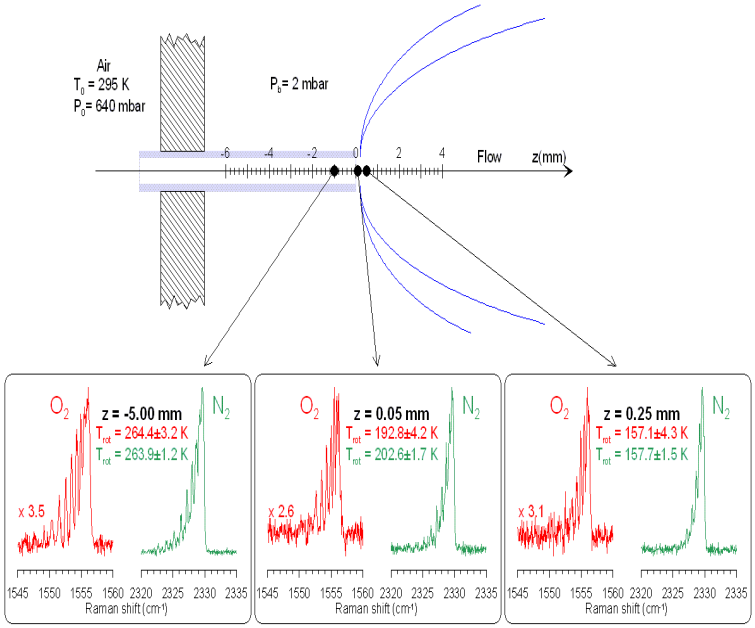


Fig. 1. Supersonic free jet of air at T_0=295 K and P_0= 640 mbar through a glass channel (inner section of 0.4x0.4 mm^2). The Raman spectra of the vibrational bands of oxygen and nitrogen at points z=-5.00 mm (inside the channel) and z= +0.05 and +0.25 mm (in the jet) and derived rotational temperatures.

ACKNOWLEDGEMENTS

This work has been supported by the Spanish MCIN/AEI/10.13039/501100011033/through grants No. PID2021-123752NB-I00.

REFERENCES

[1] S. Montero, B. Maté, G. Tejeda, J. M. Fernández and A. Ramos, *Atomic and Molecular Beams. The State of the Art 2000* (Springer, Berlin 2001), pp. 295-306.

[2] https://www.iem.csic.es/fismol/fdm/publications.html

[3] S. Bajic, *Thermométrie par marquage moléculaire pour les micro-écoulements gazeux* (Ph.D. thesis, Université Toulouse 3 - Paul Sabatier, 2023)

Experimental Evidence for the Normal Shock Instability in a Two-dimensional Granular Gas

E. Suarez Morales[1,a)], F. Zangene,[1] and M. I. Radulescu[1]

[1]*Department of Mechanical Engineering, University of Ottawa, Ottawa, ON K1N6N5, Canada.*

[a)]Corresponding author: esuar005@uottawa.ca

Shock waves in granular gases occur when particles collectively impact a wall [1]. The study of shock waves in granular gases offers the opportunity to probe the non-equilibrium structure of gaseous shock waves in the hypersonic limit. Numerical simulations of shock waves in granular gases using molecular dyamics and continuum equations have revealed a hydrodynamic instability of wavelength comparable to the shock thickness [2]. To date, this instability has not been reported in experiments and its origin remains unclear. The goal of the present study is to isolate shock waves in granular gases and characterize the shock instability.

In this work, we designed an experimental setup consisting of a gravity chute flow in a narrow channel, enabling quasi-two-dimensional particle dynamics. The experimental configuration was designed such that the channel inclination angle could be varied from 90° to 30°. Repeated experiments were conducted over a range of conditions. In each run, approximately 10^5 spherical steel beads of 1 mm diameter were released from a hopper and allowed to free-fall through the channel. Upon impact and reflection from the bottom plate, the particles rapidly compacted, producing a normal-shock configuration. The process was recorded using a Phantom v1210 high-speed camera at a resolution of 1280 $px \times 800$ px and an inter-frame time of 100 µs. Figure 1 (top) shows a representative frame. The experiments revealed a corrugation instability with a wavelength comparable to the shock thickness, in qualitative agreement with the numerical predictions of Sirmas and Radulescu [2] (Fig. 1, bottom). Furthermore, detailed particle tracking was performed to measure particle kinematics before and after shock formation, enabling the determination of local mean velocity, number density, and granular temperature. The analysis showed that regions where particles cluster exhibit a reduced granular temperature relative to neighbouring regions. The associated decrease in granular pressure produces a pressure gradient directed toward the clustered zone, which in turn draws in additional particles and amplifies the clustering.

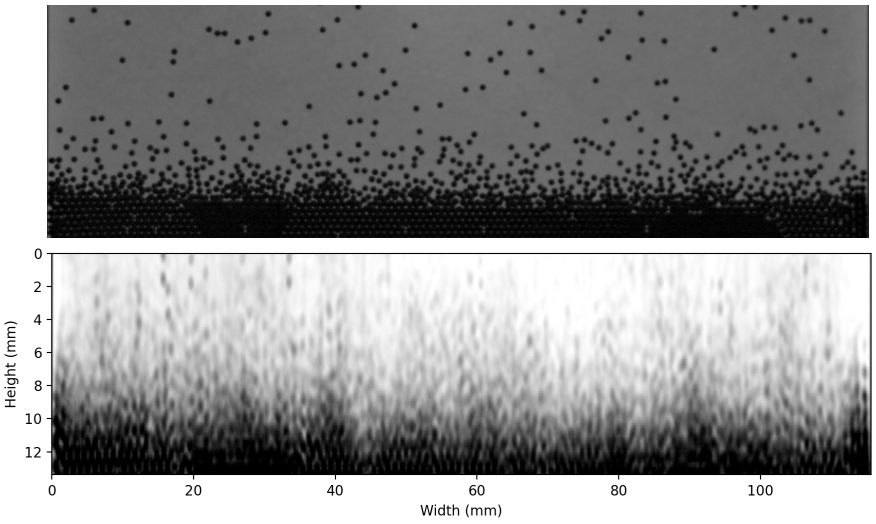


Fig. 1. Top: A single frame from direct visualization of the beads falling at an inclination of 80°**; Bottom: Overlaid and intensity-averaged shock-aligned sequence over a time window comparable to the particle crossing time.**

ACKNOWLEDGEMENTS

This work was supported by AFOSR grant FA9550-23-1-0214, with Dr. Chiping Li as program manager.

REFERENCES

[1] E. C. Rericha, C. Bizon, M. D. Shattuck, H. L. Swinney, *Physical review letters* **88**, 014302 (2001).
[2] N. Sirmas, M. I. Radulescu, *Journal of Fluid Mechanics* **873**, 568–607 (2019).

A novel two-fluid approach for modelling the near-wall collisionless electron sheath under strong thermionic emission

S. Imran[1,a)], V. Wheatley,[1] and D. I. Pullin[2]

[1]*Centre for Hypersonics, The University of Queensland, Australia*
[2]*The Lynn Booth & Kent Kresa Department of Aerospace, California Institute of Technology, USA*

[a)]Corresponding author: s.imran@uq.edu.au

In recent work, we detailed an approach for modelling the near-wall electron plasma sheath using flux boundary conditions and a fluid representation of the electrons, where the space-charge limiting effect was handled phenomenologically by introducing an analytical term to the emission fluxes [1]. In this study, we show electrostatic, particle-in-cell (PIC) simulations [2] of a 1D diode test case in the collisionless regime, where there is strong thermionic emission of electrons at the cathode. As electrons are emitted, the build-up of space charge in the region near the cathode creates a localised drop in the electrostatic potential, known as a virtual-cathode, which acts to decelerate emitted electrons and limit the current. A well-known result that is evident in the PIC simulations is that there exist two streams of electrons – a transmitted stream consisting of particles from the emitted distribution with enough energy to overcome the virtual-cathode potential, and a reflected stream of those that are not able to overcome the potential, directed back into the wall. This is an inherently kinetic effect, which is difficult to model using continuum fluid codes. To alleviate this difficulty, we propose a two-fluid model, where the forward going and reflected electron populations are represented as distinct fluid species, with exchange between the species done through a spatially varying source-term that depends only on local cell-centred values. Results of the 1D diode test case using this new model show good agreement with the PIC simulations. Finally, we discuss application of this model in our multi-fluid plasma code, Cerberus [3], to model weakly ionised hypersonic flows with electron emission from surfaces.

ACKNOWLEDGEMENTS

This research used the open-source particle-in-cell code WarpX. Primary WarpX contributors are with LBNL, LLNL, CEA-LIDYL, SLAC, DESY, CERN, Helion Energy, and TAE Technologies. We acknowledge all WarpX contributors.

REFERENCES

[1] S. Imran, D. I. Pullin, and V. Wheatley., Thermionic electron emission boundary conditions for hypersonic flow adapted to the presence of a near-surface virtual cathode, Proceedings of the 35th International Symposium on Shockwaves (submitted) Brisbane, QLD (2025)

[2] J.-L. Vay et al., WarpX: An advanced Particle-In-Cell code. DOI:10.5281/zenodo.4571577, https://blast-warpx.github.io (2018)

[3] Bond, D., Imran, S., Tapinou, K. C. and Wheatley, V.: Cerberus multi-fluid plasma simulation code, https://github.com/plasmasimuq/cerberus

Evaporation of a metal droplet in rarefied gas

D. Kalempa[1,a)] and **F. Sharipov**[2]

[1]*Departamento de Ciências Básicas e Ambientais, Escola de Engenharia de Lorena, Universidade de São Paulo, Lorena, 12602-810, Brazil*
[2]*Departamento de Física, Universidade Federal do Paraná, Caixa Postal 19044, Curitiba, 81531-980, Brazil*

[a)]Corresponding author: kalempa@usp.br

Modeling the evaporation of metal droplets in a rarefied gas is essential for accurately describing processes involving molten metals. In such systems, the metal evaporates into a mixture consisting of its own vapor and a background non-condensable gas. The evaporation rate and the associated energy flux depend on several parameters, including temperature, mixture pressure, gas composition, and the degree of rarefaction. Non-equilibrium phenomena arising in the vicinity of the droplet surface, more specifically within the Knudsen layer, can be properly described using methods of rarefied gas dynamics, such as the Direct Simulation Monte Carlo (DSMC) method or numerical solutions of the Boltzmann kinetic equation. Numerous studies have investigated evaporation and condensation processes in pure vapor and in vapor–non-condensable gas mixtures within the framework of kinetic gas theory (e.g., Refs. [1–3]). However, these studies commonly rely on the hard-sphere model of intermolecular interactions and assume hypothetical molecular masses, which may not adequately represent the complexity of real intermolecular forces. In the present work, we model the evaporation of a copper droplet in argon at a temperature of 2000 K using a kinetic model based on the linearized Boltzmann equation for a binary mixture. As in our previous study [4], the McCormack model is employed under the assumptions of complete condensation and equilibrium evaporation at the droplet surface. Interatomic interactions are described using *ab initio* potentials for argon–argon, copper–copper, and copper–argon collisions. The problem is solved numerically using the discrete velocity method over a wide range of rarefaction parameter, which depends on the mixture pressure, its temperature, and droplet radius. The mass and energy fluxes from the droplet are calculated for various degrees of gas rarefaction and molar fractions of argon in the vapor–gas mixture.

ACKNOWLEDGEMENTS

D. Kalempa acknowledges FAPESP (Fundação de Amparo à Pesquisa do Estado de São Paulo), Brazil for the support of the research, grant 2022/10476-1. F. Sharipov acknowledges CNPq (Conselho Nacional de Desenvolvimento Científico e Tecnológico), Brazil , grant 303429/2022-4.

REFERENCES

[1] Y.-P. Pao, *Phys. Fluids* **14**, 306–312 (1971).
[2] K. Aoki, S. Takata, S. Kosuge, *Phys. Fluids* **10**, 1519–1533 (1998).
[3] C. E. Siewert, *Eur. J. Mech. B/Fluids* **22**, 391–408 (2003).
[4] D. Kalempa, F. Sharipov, I. Graur, *Int.J. Heat Mass Transfer* **256**, 128021 (2026).

On the De-excitation Shock in a Hypersonic Prandtl-Meyer Nonequilibrium Oxygen Flow

A. Khraibut[1,a)] and S. L. Gai[2]

[1]*ICTP, Italy*
[2]*The University of New South Wales, Australia*

[a)]Corresponding author: akhraibu@ictp.it

Thermochemical nonequilibrium affects the aerody namic characteristics of hypersonic and re-entry vehicles. Theoretical studies of nonequilibrium have usually been conducted using simple conical geometries, enabling quantitative predictions of the flow. Experimental validation of theoretical nonequilibrium models was carried out by [1] but is limited. The experiments, however, did not observe a de-excitation shock as predicted by analytical models. In this study, we consider nonequilibrium hypersonic flow with viscous effects present in a wedge flat-plate afterbody geometry. In this geometry, thermochemical effects are produced behind the corner, which then rapidly expands the flow (through Prandtl-Meyer expansion), thereby relaxing nonequilibrium effects.

Nonequilibrium flows behind a wedge have been investigated in several studies by [2, 3, 4, 5, 6], while the structure of nonequilibrium Prandtl-Meyer flow has been analytically investigated by [7, 8, 9, 10]. However, these studies assumed a uniform flow in an equilibrium state frozen at the corner and ignored the effect of transport properties such as viscosity, thermal conductivity, and diffusion.

The model used in the present study is based on the large-scale model of [1] with wedge thickness $t = 101.6$ mm and angle $\theta = 42.5°$, sufficiently large to produce thermochemical nonequilibrium effects behind an attached shock.

In the present study, the Stochastic Parallel Rarefied Gas Time Accurate Analyzer (SPARTA) from Sandia National Laboratories, USA, has been used to obtain DSMC solutions. SPARTA is an open-source, parallelised solver that allows 2D, axisymmetric, and 3D simulations to be performed. The code uses multi-level rectilinear grids with cut/split embedding of the surface elements. The computational domain is usually constructed so that lower-order (parent) grids contain minimal information, and higher-order (child) grids include only data that allow particles to translate across cell volumes.

Results and Discussion will be given in the final paper.

Acknowledgements

The authors thank the Kuwait Foundation for the Advancement of Sciences (KFAS) for their support and HPC Cineca in Italy for providing computational resources.

References

[1] R. J. Vidal and F. Stoddard. Measurements of nonequilibrium effects in air on wedge-flat-plate afterbody pressures. techreport NASA CR-328, Cornell Aeronautical Laboratory, Inc. for Langley Reseach Center, Langley Research Center, 1965.

[2] W. G. Vincenti. Méchanique, 1:193, 1962. Linearized

[3] R. Capiaux and M. Washington. Nonequilibrium flow past a wedge. AIAA Journal, 1(3):650Ž013660, 1963.

[4] J. C. South Jr. Application of the method of integral relations to supersonic nonequilibrium flow past wedges and cones. Tech Report TR R-205, NASA, Langley Research Center, 1964.

[5] R. S. Lee. A unified analysis of supersonic nonequilibrium flow over a wedge. i-vibrational nonequi- librium. AIAA Journal, 2(4):637Ž013646, April 1964.

[6] D. J. Kewley and H. G. Hornung. Non-equilibrium dissociating nitrogen flow over a wedge. Journal of Fluid Mechanics, 64(4):725Ž013736, July 1974.

[7] W. W. Wood and J. G. Kirkwood. Characteristic equations for reactive flow. The Journal of Chem- ical Physics, 27(2):596Ž013596, August 1957.

[8] W. W. Wood and J. G. Kirkwood. Hydrodynamics of a reacting and relaxing fluid. Journal of Applied Physics, 28(4):395Ž013398, April 1957.

[9] W. W. Wood and F. R. Parker. Structure of a centered rarefaction wave in a relaxing gas. The Physics of Fluids, 1(3):230Ž013241, November 1958.

[10] J. W. Cleaver. The two-dimensional flow of an ideal dissociating gas. Technical report, The College of Aeronautics, 1959.

Abstract 196

Collisional relaxation kinetics of CO_2 at high temperature by Raman spectroscopy

C. Alvarez[1], G. Tejeda[1], and **J. M. Fernández**[1,a)]

[1] *Laboratory of Molecular Fluid Dynamics, Instituto de Estructura de la Materia, IEM-CSIC, Madrid, Spain.*

[a)] Corresponding author: jm.fernandez@csic.es

The collisional relaxation of carbon dioxide (CO_2) is present in several scientific problems of interest. These span from the radiative balance of Earth's or Mars' atmospheres [1] and the entry of space crafts [2], to the operation of the CO_2 laser [3] and of cold plasmas for fuel production [4], to name a few. The kinetics of such relaxation can be studied in the laboratory by means of supersonic gas jets, media where the gas is under non-local thermodynamic equilibrium (n-LTE) conditions [5]. In this work, a series of supersonic jets of CO_2 has been produced from high-temperature nozzles, and the gas flows have been probed by means of Raman spectroscopy with high spatial resolution. This allows to track the time evolution of the internal populations (both rotational and vibrational) resulting from the inelastic collisions between molecules.

A dedicated gas injector, able to reach temperatures up to 1000 K, was designed and built [6]. Sixteen supersonic jets of CO_2 have been analyzed, with stagnation temperatures between 298 and 1073 K, and pressures between 0.3 and 1.7 bar, from circular nozzles with 0.25 and 0.4 mm diameters. Rotational and vibrational Raman spectra have been recorded at a dense grid of discrete points along the axis of those supersonic jets. From these spectra, a precise picture of the flow quantities of the jets, and of their evolution, can be obtained. In particular, the number density, and the rotational and vibrational temperatures and populations along the gas flow have been obtained as primary quantities. From these well-determined quantities, others like the translational temperature and the flow velocity can be derived through the conservation of enthalpy and momentum. Non equilibrium statistical thermodynamics allows to retrieve macroscopic quantities like the heat capacity ratio or the increment of the entropy. All these constitute a rather complete characterization of the gas flow along the jet.

Finally, the molecular relaxation by inelastic collisions has been analyzed with a kinetic formalism, employing a Master Equation to describe the time evolution of the rotational and vibrational populations. We have obtained that way the state-to-state rate coefficients that describe the rotational relaxation kinetics of CO_2 by inelastic collisions in the thermal range from 50 to 700 K [7]. Preliminary results of the rate coefficients for the vibrational relaxation will also be presented. From these elementary rate coefficients, other macroscopic quantities such as the rotational relaxation times, the rotational relaxation cross section, and the rotational or vibrational contributions to the bulk viscosity, can be derived.

ACKNOWLEDGEMENTS

This work has been supported by the Spanish MCIN/AEI/10.13039/501100011033/ through grant No. PID2021-123752NB-I00. CA thanks the Spanish MCIN/AEI for a predoctoral grant PRE2018-085960.

REFERENCES

[1] B. Funke, M. Lopez-Puertas, M. Garcia-Comas, M. Kaufmann, M. Hopfner, and G. P. Stiller, Journal of Quantitative Spectroscopy and Radiative Transfer **113**, 1771 (2012).
[2] I. Armenise, P. Reynier, and E. Kustova, Journal of Thermophysics and Heat Transfer **30**, 705 (2016).
[3] R. L. Taylor and S. Bitterman, Reviews of Modern Physics **41**, 26 (1969).
[4] A. George, B. Shen, M. Craven, Y. Wang, D. Kang, C. Wu, and X. Tu, Renewable Sustainable Energy Review **135**, 109702 (2021).
[5] S. Montero, G. Tejeda, and J. M. Fernández, Astrophysical Journal Supplement Series **247**:14 (2020).
[6] C. Alvarez, *Estudio de la Relajación Colisional del Dióxido de Carbono a Alta Temperatura mediante Espectroscopía Raman* (Ph.D. thesis, Universidad Complutense de Madrid 2025).
[7] C. Alvarez, G. Tejeda, and J. M. Fernández, Journal of Chemical Physics **160**, 164307 (2024).

Abstract 198

Molecular Beam Experiment of Water Molecules Evaporating From a Liquid Surface at Various Temperatures

A. Fujita[1,a)], K. Sato[1], I. Kinefuchi[2]

[1] *Department of Mechanical Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*
[2] *Department of Human and Engineered Environmental Studies, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa-shi, Chiba 277-8563, Japan*

a) Corresponding author: fujita@mnf.t.u-tokyo.ac.jp

Water evaporation is a fundamental phenomenon in nature and in industrial processes. To analyze multiphase flows with phase change, it is necessary to consider the Knudsen layer in the vicinity of an evaporating surface, extending several mean free paths. The Knudsen layer shows strong nonequilibrium due to evaporation and condensation, and the functional form of the velocity distribution of molecules crossing the liquid-side boundary of the Knudsen layer remains unknown. Several theoretical models have been proposed [1, 2] to estimate the evaporative mass flux by assuming that molecules leaving the liquid phase obey the Maxwell–Boltzmann distribution, which represents the equilibrium state. By examining the actual velocity distribution of evaporating molecules and rigorously evaluating this assumption, it is expected that the mass, momentum, and energy transfer at a liquid–vapor interface can be evaluated more accurately.

In the present study, we generated the molecular beams of evaporating water molecules at various temperatures and obtained the time-of-flight (TOF) distributions of water molecules after evaporation before reaching equilibrium. The velocity distributions were obtained from the TOF distributions. The TOF distributions of evaporating molecules shifted slightly toward shorter times as the temperature increased. The velocity distributions derived from TOF distributions differed from the half Maxwell–Boltzmann distributions at the corresponding temperatures, showing a tendency toward relatively fewer slow molecules. This tendency became more pronounced as the temperature increased.

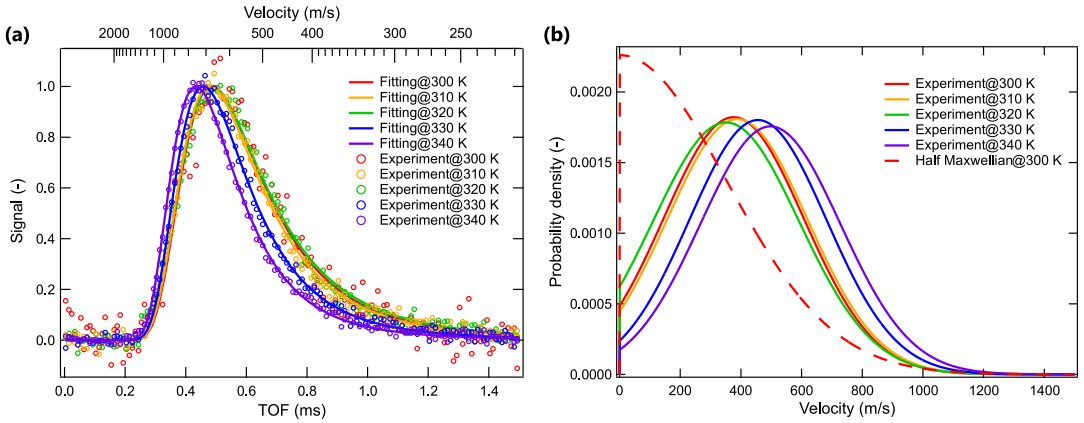


Fig. 1. (a) The TOF distributions of evaporating water molecules at various temperatures. (b) The velocity distributions obtained from the TOF distributions.

ACKNOWLEDGEMENTS

This work was supported by JSPS KAKENHI Grant Numbers JP23K26033 and JP25K21678.

REFERENCES

[1] H. Hertz, *Annalen der Physik*, **253**, pp. 177–193 (1882).
[2] Robert W. Schrage, *A Theoretical Study of Interphase Mass Transfer* (Columbia University Press, New York, 1953).

Abstract 199

Particle Merge Strategies for PIC/DSMC Plasmas

W. J. McDoniel[1,a)], A. L. Zimmer[2], C. H. Moore[1], and A. S. Fierro[2]

[1] *Sandia National Laboratories, New Mexico, USA*
[2] *New Mexico Institute of Mining and Technology, New Mexico, USA*

[a)] Corresponding author: wmcdoni@sandia.gov

Sandia's EMPIRE code [1] is often used for simulations of electron transport through a dense neutral gas with applied fields up to ~GV/m. As collisions occur, a plasma forms and the number of electrons and ions in the simulation domain grows rapidly. In some cases, the electric field even accelerates newly ionized electrons sufficiently to produce further ionization events, resulting in an avalanche. To deal with this, PIC codes typically implement some method of controlling particle counts by merging particles. Many such algorithms have been published, which have properties such as preserving different aspects of the original spatial and velocity distribution functions, and which demonstrate desirable behaviors in various test problems.

We seek to understand the behavior of various merge algorithms in environments that resemble those our users care about, as well as the effects of parameter choices for those algorithms. The goal is to have suitable merges for different applications and to recommend parameter choices (or set sensible defaults). We characterize the error produced by different algorithms and by different choices of parameter for each. We study a simple roulette merge, an instant and non-conservative re-merge for neutrals after non-ionizing collisions, a momentum-conserving 2-1 merge that selects near-neighbors in velocity space [2], and a momentum- and energy-conserving M-to-2 merge [3]. We vary parameters such as merge frequency, the threshold particle count at which we merge, and the use and aggressiveness of binning particles in velocity space.

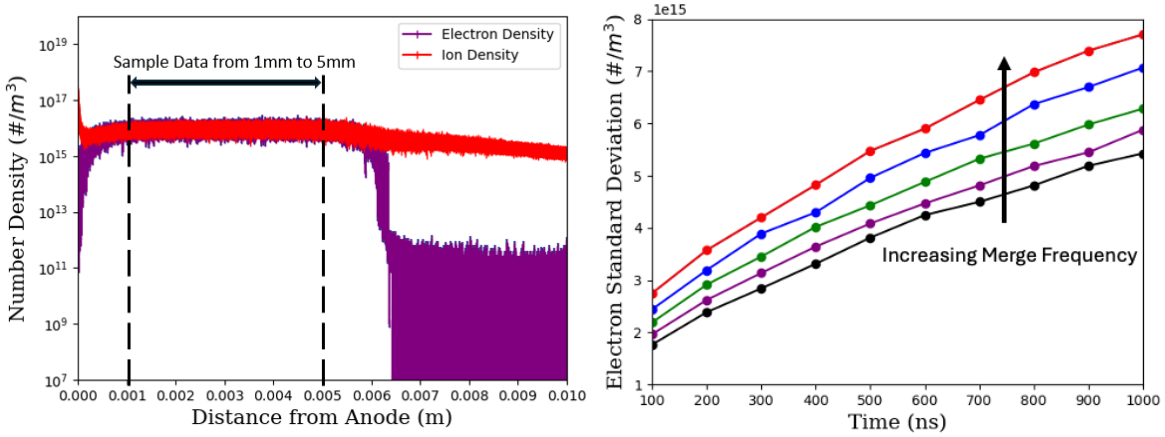


Fig. 1. A simple roulette merge applied to the plasma formed near an anode. (left) The roughly steady region we sample from. (right) The standard deviation of electron number density in that region, where the noise grows worse over time with more aggressive merges.

ACKNOWLEDGEMENTS

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

REFERENCES

[1] M. T. Bettencourt, et al., "EMPIRE-PIC: a Performance Portable Unstructured Particle-in-Cell Code." *Communications in Computational Physics*, **30** (2021).
[2] J. J. Boerner, et al., "A Performant Energy-Conserving Particle Reweighting Method for Particle-in-Cell Simulations." *Journal of Computational Physics*, **521** (2025).
[3] M. Vranic, et al. "Particle Merging Algorithm for PIC Codes." *Computer Physics Communications*, **191** (2015).

Rarefaction-Controlled Oxidizer Transport and Thermal Response in Ablating Porous Composite TPS

U. Yadav[1,a)], M. Panesi,[1] and K. Stephani[1]

[1]*Department of Mechanical and Aerospace Engineering, University of California, Irvine, CA 92697, USA.*

[a)]Corresponding author: upendray@uci.edu

Ablation of porous composite thermal protection systems is governed by competition between oxidizer delivery through the pore network and heterogeneous consumption on evolving internal surfaces. As the mean free path approaches the inter-fiber gap, rarefaction shifts transport into the transition/free-molecular regimes and can decouple local pore velocity from net oxidizer flux. Motivated by microstructure-resolved studies that characterize pore rarefaction using an inter-fiber length scale [1], we consider both uniform and nonuniform fibrous beds as idealized yet manufacturing-relevant composite microstructures. In the nonuniform case, spacing variability creates a distribution of pore throats (bottlenecks) that governs oxidizer access and penetration. We perform microstructure-resolved direct simulation Monte Carlo (DSMC) simulations using the SPARTA DSMC code and couple them, where needed, to OpenFOAM (finite-volume heat conduction) for conjugate heat-transfer analysis. For the nonuniform case, we compare oxygen-driven oxidation under identical inflow conditions in two microstructures: (i) fiber-only and (ii) fiber+matrix, where a lower-density matrix occupies inter-fiber gaps and recedes differently than the carbon fibers. With the macroscopic inflow fixed and only matrix presence varied, we quantify how phase distribution and rarefaction control near-surface oxidizer depletion, normalized number-density-gradient metrics in the fiber–matrix region, and attenuation of streamwise oxidizer number flux reaching reactive internal surfaces. For the uniform case, we couple SPARTA with OpenFOAM for conjugate heat-transfer analysis on a fixed pre-ablated fiber–matrix surface to quantify rarefaction-driven gas–solid heat transfer and resulting internal thermal non-uniformity. These results provide physics-based guidance for reduced-order ablation models that must incorporate Knudsen-dependent oxidizer transport, reaction localization, and the associated thermal response in rarefied porous media.

REFERENCES

[1] A. Y. K. Hong, M. A. Gallis, *Physics of Fluids* **37**, 096106 (2025).

Kinetic-Continuum (KC) Internal Energy and Chemistry Model for DSMC

M. D. Kroells[1,a)] and T. E. Schwartzentruber[1]

[1]*Dept. of Aerospace Engineering and Mechanics, Univ. of Minnesota, Minneapolis, MN 55455, USA*

[a)]Corresponding author: kroel012@umn.edu

In the last decade, *ab initio* simulations on high-fidelity potential-energy surfaces (PESs) have produced extensive kinetic data for air-species chemistry. Quasi-classical trajectory (QCT) and direct molecular simulation (DMS) methods, in particular, have provided reaction-rate data for the key molecular species (N_2, O_2, and NO) under both thermal equilibrium conditions (QCT) and the vibrationally depleted distributions that arise during the quasi-steady-state (QSS) dissociation stage (DMS) [1]. This progress has enabled the development of CFD dissociation models (e.g., the modified Marrone–Treanor (MMT) model [2, 3]) that incorporate *ab initio* data and closely reproduce DMS behavior [4]. However, extending comparable fidelity to DSMC is less straightforward: reaction cross-sections must be sufficiently simple to integrate to continuum rates, yet accurate enough to reproduce the targeted kinetics. Additionally, in DSMC the underlying internal energy model cannot be decoupled from the resultant thermodynamics and chemistry.

This research has two overall goals: 1) to accurately incorporate recent *ab initio* simulation data into a DSMC chemistry-modeling framework and 2) to require that the model be simple enough to allow for analytical integration in the continuum limit to ensure model consistency with CFD. To this end, we have utilized a modified version of the Kinetic-Continuum (KC) model proposed by Singh and Schwartzentruber [5]. This includes a model for internal energy with rotational-vibrational coupling via energy truncation and centrifugal barrier effects. Model parameters have been fit for five-species air and comparisons to DMS and the continuum version of the model will be presented. Figure 1 shows an example 0-D adiabatic comparison between the KC model and DMS for nitrogen.

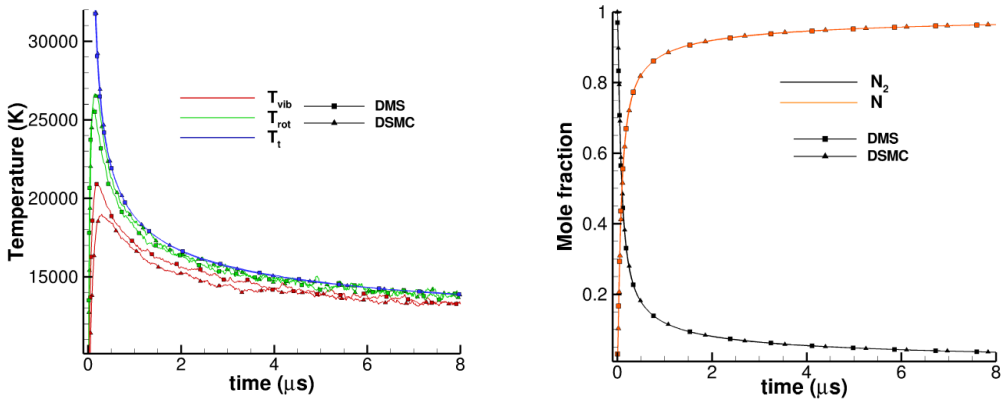


Fig. 1. Comparison of KC DSMC and DMS for 0-D adiabatic nitrogen reactor, showing temperatures (left) and mole fractions (right).

ACKNOWLEDGEMENTS

This research is funded by the AFOSR under grant FA9550-23-1-0446 and FA9550-23-1-0162.

REFERENCES

[1] E. Torres, E. C. Geistfeld, T. E. Schwartzentruber, *Journal of Thermophysics and Heat Transfer* **38**, 260–291 (2024).
[2] R. S. Chaudhry, E. Torres, T. E. Schwartzentruber, G. V. Candler, *arXiv e-prints* (2025), arXiv:2506.06236 .
[3] E. Torres, T. Gross, G. V. Candler, T. E. Schwartzentruber, *arXiv e-prints* (2025), arXiv:2506.20521 .
[4] T. Gross, *Verification and Validation of Hypersonic Air Chemistry Models in a Reflected Shock Tunnel Facility* (Ph.D. thesis, University of Minnesota, 2024).
[5] N. Singh, T. Schwartzentruber, *The Journal of Chemical Physics* **152**, 22430206 (2020).

Derivation of the generalized SO13 higher-order transport equation for non-continuum flows

Upendra Yadav* and Amit Agrawal†

* Department of Mechanical Engineering
Indian Institute of Technology (IIT) Bombay, Powai
Mumbai 400076, India
e-mail: upendra.yadav001@gmail.com

† Department of Mechanical Engineering
Indian Institute of Technology (IIT) Bombay, Powai
Mumbai 400076, India
e-mail: amit.agrawal@iitb.ac.in, web page: https://en.wikipedia.org/wiki/Amit_Agrawal

ABSTRACT

Our research group focuses on deriving higher-order transport equations for modelling flows in the transition flow regime (Knudsen number of order unity). This is pertinent since the Navier-Stokes equations do not yield accurate results in the slip- and transition-flow regimes. Whereas several approaches for deriving higher-order transport equations have been proposed in the literature, they are not entirely successful [1].

In this context, we derive the higher-order SO13 transport equations starting from the Boltzmann equation using a second-order accurate distribution function within the 13-moment framework [2]. The equations are shown to be unconditionally linearly stable and consistent with Onsager's symmetry principle. We also show that the equations comply with the second law of thermodynamics. The force-driven Poiseuille flow problem is solved analytically to establish the validity of the derived equations, and results compared against the Navier–Stokes, R13, Grad solutions and direct simulation Monte Carlo data. The proposed solution captures key rarefaction effects, including the Knudsen layer, non-uniform bimodal pressure profile, non-Fourier heat flux and the characteristic temperature dip at the centre. The analytical solution for the field variables indicates that the equations outperform the existing models in the slip- and transition-flow regimes for the problem considered.

We further derive a generalized higher-order heat transport equation and again obtain good results against benchmark data [3]. These satisfactory results point to the accuracy and applicability of the proposed equations, and the equations hold significant promise for rarefied gas dynamics at large Knudsen numbers.

REFERENCES

[1] Agrawal, A., Kushwaha, H. and Jadhav, R., *Microscale Flow and Heat Transfer: Mathematical Modelling and Flow Physics*, Mechanical Engineering Series, Springer, pp. 365, 2020.

[2] Yadav, U., Jadhav, R.S., Agrawal, A., "Derivation of linearly stable Onsager symmetric principle consistent equations and their validation for force-driven Poiseuille flow," *Journal of Fluid Mechanics*, Vol. 1020, A31 (27 pp), 2025.

[3] Yadav, U., Goutham, C.N.S., Meshram, K., Pathak, A., Bansal, D., Agrawal, A., "Derivation of the generalized heat transport equation, validation, thermodynamic consistency, and comparison with existing models," *Physical Review Applied* (to appear) 2026.

Development of Research Concepts Based on Hypersonic Wind Tunnel Experiments

O. Imamura[1,a)]

[1] *College of Industrial Technology, Nihon University, 1-2-1 Izumicho, Narashino, Chiba 275-8575, Japan*

[a)] Corresponding author: imamura.osamu@nihon-u.ac.jp

The hypersonic high-enthalpy wind tunnel in Kashiwa Campus the University of Tokyo can generate a Mach 7 airflow for approximately 60 seconds and its nozzle exit diameter is 200 mm. Figure 1 shows an overall view of the Kashiwa wind tunnel[1], with the hypersonic wind tunnel on the right. The characteristic of this wind tunnel is that students can use it relatively freely and it also allows researchers to try out their own ideas. Professor Kojiro Suzuki made immense contributions to both the installation of this facility and the research conducted within it. Figure 2 shows Professor Suzuki explaining the mechanism of the heater in the Kashiwa wind tunnel to the press at the time the wind tunnel was being set up. While the shape of hypersonic vehicle has been researched in the facility, unconventional models have also been tested, such as a paper airplane, ice body, etc. The author conducted various experiments with Professor Suzuki during initial phase of the wind tunnel setup, and here provide a brief overview of these experiments and the research concepts that were derived from them. The hypersonic wind tunnel experiments of airplane were carried out at the beginning of 2008, this experiment was an indicator of whether a paper airplane could reach the Earth's surface without burning when launched from space. This result was open to the press and widely reported, but at the same time, we believe that this challenge has demonstrated to the public that the Kashiwa Wind Tunnel is a fairly challenging facility, capable of conducting unconventional experiments. This challenge was also expanded into research concepts such as thin film or flexible models. The ice body model was also tested in the wind tunnel, which aimed to observe the simulated phoneme of the atmospheric entry of a comet[2]. In this experiment, we observed not spallation but also ice recrystallization, which was not initially anticipated, and this reaffirmed the importance of experimental research. The project also attracted the interest of many science researchers and after that the wind tunnel provided experimental opportunity not only to engineers but also to science researchers.



Fig. 1. Overview of UT-Kashiwa hypersonic and high-enthalpy wind tunnel (The right hand side is hypersonic wind tunnel.)



Fig. 2. Professor Suzuki explaining the principles of the wind tunnel heater.

REFERENCES

[1] https://daedalus.k.u-tokyo.ac.jp/wt/

[2] Osamu Imamura, Takeo Okunuki, Kojiro Suzuki, A study on ablation behavior of spherical ice piece in hypersonic flow, 10th AIAA/ASME Joint Thermophysics and Heat Transfer Conference, (2010) DOI : 10.2514/6.2010-4512

Fluid Mechanics of Evaporating and Condensing Microdroplets in the Continuum-Slip Transition Regime

E. Zabalegui Lopez[1,a)], E. Vorozhbit[1], J. Meza Galvin[1] and A. Alexeenko[1]

[1]*Purdue University, USA*

[a)]Corresponding author: ezabaleg@purdue.edu

This study investigates the fluid mechanics of micron and submicron-sized water droplets moving relative to nitrogen gas in the low Reynolds number regime, accounting for evaporation and condensation effects from the droplet surface and non-negligible rarefaction effects. The motivation stems from Rapid Depressurization-Controlled Ice Nucleation (RD-CIN), a freeze-drying technique in which supercooled droplets are generated in vial headspace following rapid pressure reduction. During depressurization, droplets accelerate relative to a predominantly nitrogen environment (at or near atmospheric pressure), while simultaneously undergoing mass transfer effects due to the relative humidity of the carrier gas. Although the bulk gas is not dilute and remains near atmospheric density, micron-scale droplet diameters can produce Knudsen numbers approaching or exceeding Kn = 0.01, placing the system in the slip-flow regime, while Re ¡ 1 leads to Stokes flow due to the small relative velocity of the droplets and their size. Under these conditions, classical continuum correlations for Stokes drag and heat transfer become insufficient, particularly when coupled with interfacial mass flux driven by vapor pressure differences and temperature gradients. The resulting momentum exchange is further modified by Stefan flow and thermal accommodation effects at the droplet surface. This work compares Direct Simulation Monte Carlo (DSMC) and continuum CFD predictions for evaporating and condensing droplets in the continuum-to-slip transition regime across different droplet radii (10^{-8}– 10^{-4} m) and humidity levels. In addition to DSMC, a deterministic solution of the Boltzmann equation using a Discontinuous Galerkin Fast Spectral (DGFS) solver is employed, providing a noise-free kinetic reference that is particularly well suited for low-speed flows, where statistical noise in DSMC can affect accuracy. The continuum simulations solve the creeping-flow Navier2̌013Stokes equations using three surface boundary conditions: no-slip, Maxwell slip, and slip with interfacial mass transfer. Rarefaction effects are incorporated through slip corrections, while evaporation and condensation are modeled via vapor-pressure-driven mass flux coupled to heat transfer. By imposing identical Reynolds and Knudsen numbers across continuum and kinetic approaches, deviations between CFD, DSMC, and DGFS are quantified. The results clarify the conditions under which continuum CFD remains predictive and identify regimes where particle-based modeling becomes necessary for accurate droplet dynamics. Collectively, these findings improve predictive capability for droplet trajectories in RD-CIN processes and contribute to a broader understanding of low-Reynolds-number multiphase transport under weakly rarefied conditions relevant to pharmaceutical freeze-drying and aerosol systems.

Investigating Fibre Optic Intensity Calibrations for Spectrally Resolved Surface Emission Spectroscopy of Non-Equilibrium Flows

R. C. Hawken[1,a)], S. G. Lock[1] and C. M. James.[1]

[1]*Centre for Hypersonics, School of Mechanical and Mining Engineering, The University of Queensland, St Lucia, QLD, 4072, Australia.*

[a)]Corresponding author: r.hawken@uq.edu.au

During atmospheric entry, shock-layer temperatures can exceed 10,000 K, but only a fraction of this energy radiates to the vehicle surface. While radiometers measure peak radiative heat flux, they do not resolve the atomic and molecular sources of this radiation, which are instead inferred from computational fluid dynamics (CFD) chemical models [1]. A key challenge remains to characterise the spectral nature of radiative heating at the surface. Emission spectroscopy identifies radiating species within the hypersonic shock layer; however, conventional systems observe the entire flow field externally, making it difficult to determine the radiative heat flux incident on the vehicle surface [1].

A motivating case for developing an improved surface radiation spectral measurement technique is the upcoming NASA Dragonfly mission to Saturn's moon Titan, launching in July 2028 and arriving in 2035. This mission involves delivering a 4.5 m diameter capsule through Titan's thick Methane and Nitrogen atmosphere, then deploying a flying octo-copter to explore the carbon-rich environment.

Preliminary CFD radiation simulations from NASA Ames estimate that the Dragonfly entry vehicle may experience up to 94% of the total forebody shoulder heating from radiative processes [2]. However, similar predictions include -50% to 200% uncertainty in post-shock species concentrations due to strong thermochemical non-equilibrium processes occurring during Titan entry [3]. The dissociation and recombination of nitrogen and methane create an abundance of CN radicals, which directly contribute to increased radiative heating across the ultraviolet, visible, and near-infrared regions [2].

Emerging studies at the University of Queensland (UQ) X2 Expansion Tube demonstrate that an optic fibre, flush-mounted on a vehicle's surface and protected by a window, can perform surface emission spectroscopy to directly measure and spectrally resolve the radiative heat flux at the surface [4]. This technique can be used to update computational modelling of hypersonic radiation codes and reduce surface radiative heat flux uncertainties. However, inconsistencies in optic fibre radiation intensities were identified during preliminary stagnation-point studies in 2023 [5] and 2024 [4] at UQ. This highlights the need for thorough investigation of intensity calibration techniques before drawing definitive conclusions. This research aims to improve the understanding of intensity calibration methods most suited to fibre-optic surface spectroscopy, enabling further investigation of Dragonfly entry heating.

The methodology of this investigation includes the development of a bench-top calibration apparatus to measure the intensity of radiation captured from a Labsphere integrating sphere used as a stable radiation source, across a range of optic fibre numerical apertures. The study also tracks how radiation intensity changes due to optic fibre bending required for model installation into the X2 tunnel for in-situ intensity calibrations. Additional variables include changes in radiation intensity with linear and lateral separation distance between the integrating sphere and optic fibres, as well as intensity variations with and without a protective window.

To progress reliably with the surface-mounted optical fibre spectroscopy technique, it is essential to thoroughly understand and document the intensity calibration process prior to experimental Titan entry testing. Understanding and mitigating transmission losses through the optic fibres will strengthen the reliability of future findings.

REFERENCES

[1] A. P. Rao, J. D. Crespo, P. Valentini, V. J. Murray, E. I. Vaughan, Z. S. Davis, R. Alviani, M. Kulakhmetov, *Journal of Spacecraft and Rockets* **62**, 1–14 (2025).

[2] C. O. Johnston, T. K. West, A. M. Brandis, *Features of Afterbody Radiative Heating for Titan Entry, AIAA Aviation 2019 Forum* (2019).

[3] A. C. Tibère-Inglesse, C. O. Johnston, A. M. Brandis, B. A. Cruden, *Backshell radiation measurements in the EAST facility for Titan entry, AIAA SciTech 2023 Forum* (2023).

[4] H. Subra, R. Allison, S. Lock, Y. Liu, M. Uren, R. Hawken, C. M. James, *Through-Model Fibre Optic Emission Spectroscopy for Studying Planetary Entry Radiative Heat Flux, 10th ESA RHTG* (2024).

[5] R. Allison, *Through-Model Fibre Optic Emission Spectroscopy in the X2 Expansion Tube* (Undergraduate thesis, The University of Queensland, 2023).

Nonequilibrium Ionization and Chemistry Effects of H_2O Plume Injection in Rarefied Hypersonic Reentry Flow

E. Zabalegui Lopez[1,a)], E. Vorozhbit[1], J. Meza Galvin[1] and A. Alexeenko[1]

[1]*Purdue University, USA*

[a)]Corresponding author: ezabaleg@purdue.edu

This work examines finite-rate chemistry and nonequilibrium ionization of air, H_2O and its dissociated species during high-altitude atmospheric reentry in the transitional flow regime (Kn $\simeq$ 0.05). Specifically, the work aims to capture the interaction of a Mach 25 bow-shock with water vapor injected near the nose of a reentry vehicle by a micro-scale thruster. The computational study is motivated by the integration of a reentry capsule with the Film Evaporation MEMS Tunable Array (FEMTA), a micro propulsion technology allowing for the vaporization of liquid water propellant. This study provides a numerical platform for designing high-enthalpy chemistry experiments that are difficult to reproduce in ground-based laboratory tests. A multi-scale DSMC approach is implemented using the SPARTA solver to characterize the micron-scale exhaust properties of the water vapor, later coupling them to the meter-scale free-stream flow around the re-entry vehicle. The simulations capture high altitude reentry capsule flow phenomenon where translational, rotational, and vibrational modes are decoupled. The study aims to quantify the impact of water vapor injection on nonequilibrium dynamics by computing multi-species chemical reaction kinetics, with adaptive meshing and adaptive timestep techniques to properly capture the shock and its interaction with the water vapor jet. Unlike common large-scale shock-plume interaction problems where the focus lies solely on the impact on the aerothermodynamics, the present study focuses on localized chemical reactions within the shock layer caused by the introduction of the water vapor into the high enthalpy flow, and the impact on ionization leading to high radiative emission.

Abstract 211

Flight Configuration Optimization of VLEO Satellites Considering Electromagnetic Forces under Strong Geomagnetic Activity

H. Ding[1,2], S. Q. Zhang[1,2], D. D. Zeng[1,2], X. L. Yu[1,2], and **S. H. Li**[1,2,a)]

[1] *State Key Laboratory of High Temperature Gas Dynamics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China.*
[2] *School of Engineering Science, University of Chinese Academy of Sciences, Beijing 100049, China.*

[a)] Corresponding author: LEE@imech.ac.cn

In the VLEO regime (100–400 km), the thermosphere is characterized by transitional to free-molecular flow. The increased neutral number density renders aerodynamic drag non-negligible and the dominant non-conservative force governing orbital decay [1]. At these altitudes, aerodynamic forces can no longer be treated as perturbations, and drag-minimizing configuration design plays a decisive role in satellite lifetime. Conventional VLEO configuration optimization is primarily based on free-molecular theory or DSMC methods [2,3], considering only neutral aerodynamic drag and heat flux effects. However, under strong geomagnetic activity, enhanced plasma density and electron temperature modify the satellite surface potential and sheath structure. The resulting electromagnetic forces significantly modify surface force distributions for different flight configurations [4], thereby affecting the overall rarefied aerodynamic forces and moments.

In this study, a coupled DSMC–PIC–MCC framework [5] is employed to simulate neutral and plasma flow fields around realistic satellite geometries. A high-fidelity multi-parameter database is constructed under varying flight environments, configurations, and surface properties. Based on these data, a multi-physics constrained surrogate model [6] is developed for VLEO configuration optimization, enabling the determination of optimal configurations and surface force distributions under different geomagnetic conditions.

Results indicate that under strong geomagnetic activity, increasing plasma density and enhanced surface potential significantly increase electromagnetic forces, which may become comparable to neutral forces under extreme conditions. Neglecting electromagnetic effects leads to substantial underestimation of total drag and torque, resulting in suboptimal flight configurations. Configurations optimized with electromagnetic effects considered achieve a maximum drag reduction of approximately 20%.

These findings demonstrate that electromagnetic forces play a critical role in determining force characteristics and optimal design parameters of VLEO satellites under strong geomagnetic activity. The present work provides a foundation for refined configuration optimization of VLEO satellites accounting for geomagnetic effects.

REFERENCES

[1] J. Zhang, Y. F. Jiang, S. Chen, S. H. Li, Overview of aerodynamic drag calculation and reduction design for very low Earth orbit satellites, *Acta Aeronaut. Astronaut. Sinica* **45** (21), 029796 (2024).
[2] G. A. Bird, Monte Carlo simulation of gas flows, *Annu. Rev. Fluid Mech*. **10** (1), pp. 11–31 (1978).
[3] C. Shen, *Rarefied Gas Dynamics* (Springer, Berlin, 2005).
[4] C. Capon, M. Brown, R. Boyce, Direct and indirect charged aerodynamic mechanisms in the ionosphere, *Adv. Space Res*. **62** (5), pp. 1090–1101 (2018).
[5] C. K. Birdsall, Particle-in-cell charged-particle simulations, plus Monte Carlo collisions with neutral atoms, PIC-MCC, *IEEE Trans. Plasma Sci*. **19** (2), pp. 65–85 (1991).
[6] M. Raissi, P. Perdikaris, and G. E. Karniadakis, Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, *J. Comput. Phys*. **378**, pp. 686–707 (2019).

Abstract 212

Influence of Polar Environment on the Orbital Dynamics of Near-Polar VLEO Satellites

S. H. Li[1,2,a)], H. Ding[1,2], S. Q. Zhang[1,2], D. D. Zeng[1,2], and H. Chen[1,2]

[1] *State Key Laboratory of High Temperature Gas Dynamics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China.*
[2] *School of Engineering Science, University of Chinese Academy of Sciences, Beijing 100049, China.*

[a)] Corresponding author: LEE@imech.ac.cn

VLEO satellites have experienced rapid growth due to their advantages in Earth observation, data transmission, and communication capacity, with the number of satellites in orbit expected to reach the million scale. Therefore, operational strategies for mega-constellations are essential. For near-polar orbits, satellites frequently traverse polar regions where the space environment is strongly influenced by geomagnetic topology, particle precipitation, and Joule heating. As a result, thermospheric density, composition, and ionization rate exhibit strong gradients and rapid variations along the orbit, leading to pronounced spatiotemporal inhomogeneity [1]. Under such conditions, neutral rarefied gas dynamics and plasma dynamics are coupled, and satellites are subjected to both neutral aerodynamic and electromagnetic forces [2–4]. The orbital dynamics therefore exhibit enhanced multi-source non-conservative perturbations and strong nonlinearity. Neglecting plasma-induced electromagnetic perturbations may lead to underestimation of non-conservative forces and their long-term impact on orbital evolution.

In this study, a DSMC–PIC–MCC numerical framework [5] is employed to simulate neutral and plasma flow fields around near-polar satellites. The aerodynamic characteristics along the orbital trajectory are analyzed, and a non-conservative force model for VLEO satellites in complex polar environments is established. This model is incorporated into the orbital dynamics equations including the J2 perturbation term [6], and a high-precision orbit propagation model applicable to polar environments is developed [7]. Based on this framework, orbital evolution characteristics are investigated under varying solar activity levels, orbital altitudes, configuration parameters, etc.

Results indicate that when electromagnetic perturbations are considered, the environmental inhomogeneity in polar regions significantly amplifies drag coefficient fluctuations, resulting in periodically enhanced semi-major axis decay rates. Moreover, electromagnetic perturbations induce cumulative deviations of the orbital plane over long-term integration. Compared with conventional propagation models, the developed high-precision model more accurately captures the orbital evolution mechanisms in polar environments.

This work provides a high-fidelity analytical framework and theoretical basis for orbital lifetime assessment, perturbation compensation design, and operational strategy optimization of near-polar VLEO mega-constellations.

REFERENCES

[1] R. W. Schunk, A. F. Nagy, *Ionospheres: Physics, Plasma Physics, and Chemistry*, 2nd ed. (Cambridge University Press, Cambridge, 2009).
[2] C. Shen, *Rarefied Gas Dynamics* (Springer, Berlin, 2005).
[3] G. A. Bird, Monte Carlo simulation of gas flows, *Annu. Rev. Fluid Mech*. **10** (1), pp. 11–31 (1978).
[4] C. Capon, M. Brown, R. Boyce, Direct and indirect charged aerodynamic mechanisms in the ionosphere, *Adv. Space Res*. **62** (5), pp. 1090–1101 (2018).
[5] C. K. Birdsall, Particle-in-cell charged-particle simulations, plus Monte Carlo collisions with neutral atoms, PIC-MCC, *IEEE Trans. Plasma Sci*. **19** (2), pp. 65–85 (1991).
[6] D. A. Vallado, *Fundamentals of Astrodynamics and Applications* (Microcosm Press, Hawthorne, 2013).
[7] M. Oliver and G. Eberhard, *Satellite Orbits: Models, Methods and Applications* (Springer, Berlin, 2012).

Abstract 214

Numerical Study of Photophoretic Forces on a Thin Plate with Various Structured Surfaces

J. Chen[1,a)], and Y.Wang[1]

[1] *Department of Mechanics, Tianjin University, Tianjin, 300072, China*
[a)] Corresponding author: jie.chen@tju.edu.cn

Photophoretic levitation has attracted increasing attention as a potential propulsion mechanism for near-space flight applications [1]. Its capability to enable sustained atmospheric measurements, enhance telecommunications, and support Martian exploration underscores its significance in aerospace engineering. Azadi et al. [2] demonstrated that macroscopic polymer films with nanostructured surfaces can achieve levitation under low-pressure conditions when illuminated by light. In their study, a Mylar film coated with carbon nanotubes on one side created a difference in accommodation coefficients between the two surfaces, thereby generating a net force under uniform heating. A comprehensive understanding of how structural properties govern photophoretic lift is essential for the development of controllable and efficient levitation systems. In this study, a thin plate with a structured surface is investigated using the direct simulation Monte Carlo (DSMC) method. The plate is maintained at a constant temperature higher than the ambient gas temperature and is immersed in a low-pressure environment. Both surfaces are assigned uniform accommodation coefficients, with a smooth top surface and a structured bottom surface. Various geometries, including rectangular, ratchet-type [3], and other representative configurations, are investigated. The results demonstrate that the net levitation force can be achieved through intensified gas–surface interactions induced by the surface structure. Moreover, a horizontal force comparable in magnitude to the levitation force can be generated by introducing a ratchet-type surface geometry, owing to the temperature difference in the surrounding gas. The effects of structural parameters, accommodation coefficient, and environmental conditions are systematically examined. These findings provide guidance for the design of controllable photophoretic levitation systems.

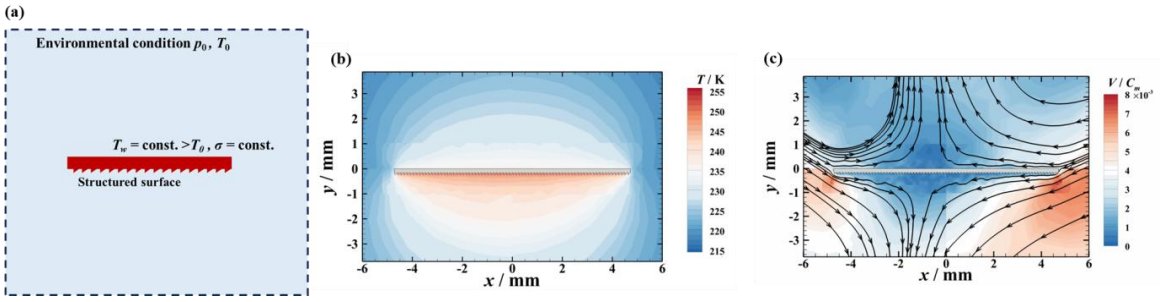


Fig. 1. Schematics diagram of computational domain (a), temperature field (b) and speed distributions with streamlines

ACKNOWLEDGEMENTS

This work was supported by the National Natural Science Foundation of China under grant number 92471106.

REFERENCES

[1] B. C. Schafer, J. Kim, *et al.*, Photophoretic flight of perforated structures in near-space conditions, *Nature*, 644, pp:362 (2025).
[2] Azadi, Mohsen, *et al.*, Controlled levitation of nanostructured thin films for sun-powered near-space flight. *Science Advances,* 7(7), pp: eabe1127 (2021).
[3] J. Chen, S. Stefanov, *et al.*, Analysis of flow induced by temperature fields in ratchet-like microchannels by Direct Monte Carlo Simulation, *International Journal of Heat and Mass Transfer*. 99, pp:672-680 (2016).

An Implicit Unified Gas-kinetic Scheme with Adaptive Mesh Refinement in Velocity Space

Q. Yuan[1,a)] and Q. Li[1]

[1]*Tsinghua University, China*

[a)]Corresponding author: yqqyspring@outlook.com

The unified gas-kinetic scheme (UGKS) is a multi-scale method for all flow regimes. However, under highly rarefied and hypersonic conditions, the requirement of wide range of velocity space and small discrete velocity interval lead to prohibitive computational cost and memory consumption, which limits its application to three-dimensional complex problems.

In this work, an efficient unified gas-kinetic scheme is proposed. A predicted equilibrium distribution is first obtained through implicit solution of the macroscopic equations, followed by an implicit solution of the evolution equation for the gas distribution function, with the lower-upper symmetric Gauss-Seidel factorization method employed to achieve fast convergence. To further enhance computational efficiency and overcome memory constraints, an octree-based adaptive mesh refinement in velocity space is implemented, utilizing the contribution to moments from numerical quadrature and the gradient of the velocity distribution function in the velocity space as adaptation criteria.

Typical flows covering the whole flow regimes are simulated using the current method. Numerical results demonstrate that the number of velocity grid points can be reduced by one to two orders of magnitude, while fast convergence is achieved with the implicit method.

Abstract 216

Wave–particle turbulent simulation (WPTS), one multi-scale non-equilibrium turbulence modeling approach

X. Yang[1,a)], and K. Xu[1]

[1] *Department of Mathematics, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong.*

[a)] Corresponding author: xyangbm@connect.ust.hk

Turbulence comprises a hierarchy of interacting flow structures across a wide range of spatial and temporal scales. The complex and nonlinear nature of these interaction renders direct numerical simulation (DNS) prohibitively expensive, highlighting the significance of research on turbulence modeling and numerical methods.

The mixing length theory proposed by Prandtl is a cornerstone of turbulence modeling. It conceptualizes small-scale eddies as discrete fluid particles, like gas molecules, migrate over a characteristic distance before exchanging momentum with their surroundings. This concept was subsequently integrated with eddy-viscosity turbulence models, leading to the modeling fundamentally rooted by diffusion processes. In this work, we proposed a novelty method, wave-particle turbulent simulation (WPTS), where large-scale turbulent structures are resolved directly using a wave-based description, while the collective effect of unresolved subgrid-scale motions is modeled via stochastic particles that represent discrete fluid parcels. WPTS thus inherits and extends the mixing length hypothesis, but has two fundamental distinctions: (1) it fully preserves the non-equilibrium transport characteristics of the particles; and (2) it unifies the evolution of these particles with the wave dynamics of the resolved background field, establishing a unified multiscale framework applicable across both turbulent and laminar regimes.

A typical feature of WPTS is its wave-particle adaptivity. The contribution of particle component is dynamically modulated by the local turbulence intensity. In regions of high turbulence intensity where the computational grid is insufficient to resolve the flow, the particles will be sampled. Conversely, in laminar regions where the flow is fully resolved on the grid, no particles are generated, and WPTS seamlessly reverts to gas-kinetic scheme (GKS), a standard Navier-Stokes solver. This adaptivity feature is clearly illustrated in Fig. 1, which shows the wave/particle components in WPTS for a spatially-developing jet flow.

Currently, the generation, advection, and annihilation of particles in WPTS are directly linked to the production and dissipation of unresolved turbulent kinetic energy within a cell. In fact, particle-level modeling holds significant promise for progressive refinement, incorporating additional degrees of freedom to further increase prediction accuracy. WPTS method has undergone preliminary validation in typical turbulence flows, including mixing layers and spatially developing jets, demonstrating its potential as a powerful tool for turbulence modeling and simulation.

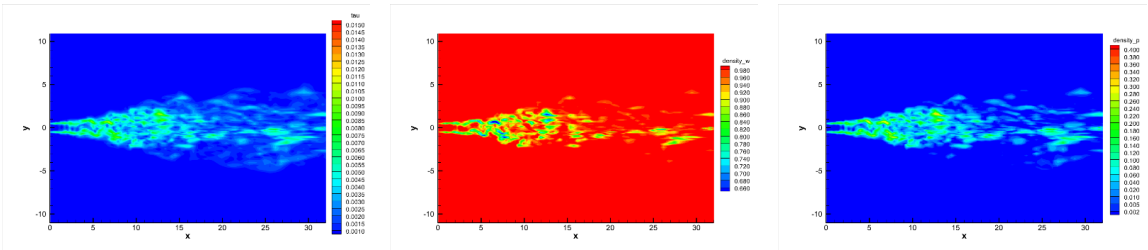


Fig. 1. The illustration of wave-particle coupling in WPTS for jet flow: (left) the modeled collision time, (middle) the wave component, (right) the particle component.

REFERENCES

[1] X. Yang, K. Xu, arXiv preprint arXiv:2503.07207 (2025).
[2] X. Yang, K. Xu, Physics of Fluids 37 (2025).
[3] X. Yang, K. Xu, arXiv preprint arXiv:2602.09759 (2026).

Abstract 218

Knudsen Force Acting on an Asymmetric Object

Tsuyoshi Makita[1, a)] and Shigeru Yonemura[2]

[1] *Department of Mechanical Engineering, Graduate School of Engineering, Chubu University, 1200 Matsumoto-cho, Kasugai, Aichi 487-8501, Japan.*
[2] *Department of Mechanical Engineering, College of Engineering, Chubu University, 1200 Matsumoto-cho, Kasugai, Aichi 487-8501, Japan.*

[a)] Corresponding author: t_makita8942@outlook.com

The Knudsen force, which arises from momentum exchange between gas molecules and solid surfaces in the transition regime, plays a significant role in micro-scale devices. This force is closely related to thermal induced flows, such as thermal edge flows, which are generated by temperature inhomogeneities near the object surfaces [1]. The objective of this study is to investigate how an asymmetric shape of object can modulate the magnitude and direction of this force.

To evaluate the Knudsen force, we employed the Direct Simulation Monte Carlo (DSMC) method [2], which is well-suited for analyzing gas flow in the transition and free-molecular regimes. The computational domain is sandwiched by two hot parallel plates, and a cold asymmetric object is placed at the center of domain. The gas-surface interaction was modeled using Maxwell's boundary condition with an accommodation coefficient of 1. Simulations were performed across a range of Knudsen numbers Kn from 0.1 to 10 to capture the peak of force. Here, the gap between the cold object and the hot plates is used as the characteristic length to define the Knudsen number Kn. Figure 1 illustrates the pressure distribution and flow velocity vectors around the asymmetric cold object at $\mathrm{Kn} = 0.1$, where P_0 is the spatially averaged pressure in the computational domain. From Fig. 1, it is found that the pressure near the leftward rounded head of the object becomes smaller than that of the surrounding gas, whereas the pressure near the rightward inclined planes is as much as that of the surrounding gas. This pressure imbalance, coupled with the reaction force of the tangential force inducing rightward gas flow along the inclined planes, results in net Knudsen force acting in the negative *x*-direction. In conclusion, this study demonstrates that an asymmetric object can generate Knudsen force by inducing local pressure imbalance in the transition regime.

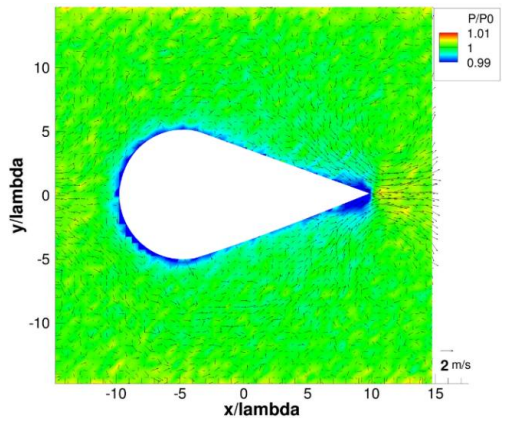


Fig. 1. Pressure distribution P/P_0 and flow field around an asymmetric cold object at $Kn = 0.1$.

REFERENCES

[1] C. J. C. Otic and S. Yonemura, *Micromachines*, **13**(7), 1092 (2022).
[2] K. Nanbu, *Reports of the Institute of Fluid Science, Tohoku University*, **3**, pp. 47-93 (1992).

Research on the Mechanism of OH Ultraviolet Non-equilibrium Radiation Spectral Characteristics in Hypersonic Rarefied Flow

S. Chai[1,a)], Y. Zhang[1], D. Zeng[1], H. Chen[1] and S. Li[1]

[1]*State Key Laboratory of High Temperature Gas Dynamics, Institute of Mechanics, Chinese Academy of Sciences, China*

[a)]Corresponding author: LEE@imech.ac.cn

During spacecraft re-entry and on-orbit flight, the interaction between hypersonic flow and wake markedly influences the vehicle's aerodynamic target characteristics. In high-temperature gas flowfields, the hydroxyl radical (OH) produced from the atmospheric and H_2O dissociation serves as a key tracer species in the complex chemical reactions within the flow and wake regions. The $A_2\Sigma^+ \leftarrow X^2\Pi$ electronic transition of OH is the dominant optical radiation source, with its peak bands located at 283 nm and 309 nm [1,2]. However, under high-temperature and strongly non-equilibrium conditions, it remains unclear how collisions between OH and other particles alter the level populations and radiative lifetimes related to the $A_2\Sigma^+ \leftarrow X^2\Pi$ electronic transition.

This study employs the self-developed non-equilibrium Atmospheric Infrared Radiation TRANsfer (AIRTRAN) model[3], to simulate the collisional excitation and radiative processes of OH with species such as N2, O_2, H, O, under various high-temperature and highly excited conditions by regulating collision processes and kinetic parameters. The ultraviolet radiation spectra of the OH $A_2\Sigma^+ \leftarrow X^2\Pi$ electronic transition band system are calculated, and the influences of collisional translational energy and vibrational-rotational level populations on the spectral intensity and distribution are quantitatively analyzed. This reveals the mechanistic link between microscopic energy transfer and the radiative spectra.

The analysis demonstrates that: (1) Under typical conditions, the ultraviolet radiation characteristics obtained in this work show good agreement with flight test data, such as from the RAM-C II experiment[4]; (2) The collisions between OH and energetic H atoms are identified as the dominant quenching mechanism for OH(A), which can significantly reduce the radiation intensity in the 283 nm and 309 nm bands; (3) By directionally regulating rate coefficients for processes such as dissociation, collisional excitation, and quenching, the spectral structure of the OH ultraviolet radiation can be significantly altered.

This study provides a theoretical foundation for the precise simulation and regulation of ultraviolet radiation in hypersonic high-temperature flowfields.

References

[1] L. Bai, D.-M. Zhang, Q. Lv, L.-L. Zhang, Y.-K. Wang, Y.-Y. Xu, J. Quant. Spectrosc. Radiat. Transfer, 271, pp. 107671 (2021).

[2] H. Zheng, and T. Bai, Optik, 165, pp. 159-167 (2018).

[3] S. Chai, D. Zeng, H. Chen, B. Yan, X. Yu, and S. Li, Proc. SPIE, 13668, pp. 1366814 (2025).

[4] W. L. Jones, and A. E. Cross. NASA Technical Note D-6617 (1972).

Abstract 222

Molecular Dynamics Study of Reactive Gas–Surface Interactions Induced by Atomic Oxygen in VLEO

Zhi-Hui Wang[1,2,a)], Rui-Ling Tao[3] , Chao-Yue Zhao[1] and Xu-Hong Jin[4]

[1] *School of Engineering Science, University of Chinese Academy of Sciences, 101408, Beijing, China*
[2] *State Key Laboratory of Nonlinear Mechanics, Chinese Academy of Sciences, 100190, Beijing, China*
[3] *Beijing Institute of Spacecraft System Engineering，100094，Beijing, China*
[4] *China Academy of Aerospace Aerodynamics, 100074, Beijing, China*

[a)] Corresponding author: wisdom@ucas.ac.cn

The development of very low Earth orbit (VLEO) spacecraft [1,2] has recently attracted increasing attention in the aerospace community. Operating in a high-speed free-molecular flow environment, the aerodynamic characteristics of such vehicles are dominated by GSIs [1], in which the momentum and energy accommodation coefficients play a critical role in design and performance prediction. Atomic oxygen, a major constituent of the VLEO atmosphere, is highly reactive and can readily adsorb onto and erode material surfaces, thereby modifying surface scattering characteristics and influencing both aerodynamic and thermal behavior, as shown by Fig. 1. Despite its importance, quantitative understanding of these effects remains limited, due in part to the extreme difficulty of conducting relevant experiments and the high computational cost of fully resolved molecular simulations. Particularly, the substantial difference in characteristic time scales between the solid and gas phases makes molecular dynamics simulations of reactive GSIs significantly more challenging than simulations of conventional pure solid or gas systems.

In this study, building on our previous studies, we propose an equivalent molecular dynamics simulation strategy that captures the essential features of atomic-oxygen-induced surface erosion and scattering processes within practical computational constraints. The simulation procedure consists of two main steps. First, the characteristic physical time scale of heat transfer within the simulated wall is evaluated, and combined with the relaxation time associated with the wall thermostat, the interval between successive high-speed atomic oxygen impacts is determined. This strategy allows the incident frequency to be increased so as to effectively reduce the computational cost, while ensuring that the wall temperature remains essentially stable, thereby preventing artificial distortion of the wall structure and properties. Under such continuous-incidence conditions, the effective duration corresponding to real GSIs in a rarefied atmospheric environment can be estimated based on the equivalence of the number of incident particles. Once a dynamically stable wall state is obtained, single-incidence simulations are then performed. In this stage, a single atomic oxygen particle is repeatedly injected with randomized initial positions and incident angles, and the resulting momentum and energy accommodation coefficients, as well as chemical reaction probabilities, are statistically evaluated for use in DSMC method. Using this methodology, we have preliminarily investigated the GSI features of several common aerospace materials, including titanium dioxide, silicon dioxide, aluminum, and polyimide. The results provide reference data that may be useful for drag prediction of new-generation VLEO spacecraft and for the intake design of air-breathing electric propulsion (ABEP) systems [2].

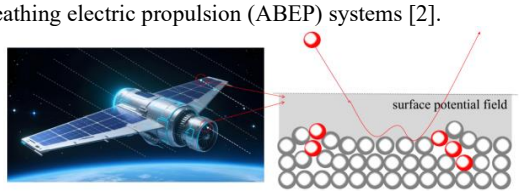


Fig. 1. Schematic diagram of gas-surface interaction in VLEO free molecular flow.

ACKNOWLEDGEMENTS

This work was supported by the Strategic Priority Research Program (B) of Chinese Academy of Sciences (grant XDB0620203).

REFERENCES

[1] S. Livadiotti, N. H. Crisp, P. C. Roberts, et al., *Progress in Aerospace Sciences*, **119**, 100675 (2020).
[2] A. S. Filatyev, A. A. Golikov, A. I. Erofeev, et al., *Progress in Aerospace Sciences*, **136**, 100877(2023).

Experimental investigation of non-thermal plasma jet chemistry

R. J. Kurian[1], N. Temme [1], F. Zare [1], C. Jacobs [1], V. Wheatley[1],

[1]*The University of Queensland, Brisbane, Australia*

Corresponding author: uqrjohnk@uq.edu.au

In the field of plasma propulsion; both air-breathing and space based plasma thrusters, the chemistry of the plasma jet is not well understood and system performance is highly dependent on the non-thermal plasma chemistry, particularly the recombination rate at high thrust densities [1]. The uncertainty in non-thermal plasma chemistry is due to the complexity of mechanisms and the difficulty in measuring detailed plasma species distributions over time. As the performance of these engines are highly dependent on the electron number density and resistance of the plasma jet, it is important to understand the recombination rates of the various species in the jet. The work presented here is to address this gap and support future computational and experimental efforts in understanding these types of jets.

The plasma jet is produced by a dielectric barrier discharge (DBD) plasma source, which is a type of non-thermal plasma source. The electrodes are separated by a quartz tube and gas is allowed to flow through the tube at 8.5 ln/min, slightly above atmospheric pressure. The plasma jet is then characterized using optical emission spectroscopy and the spectra at different locations and applied electric fields is used to determine the recombination rates of the various species in the plasma jet. This paper will study Argon, Nitrogen, and Air plasma jets at different electric fields and supply conditions. The results are compared and contrasted with existing computational models and previous experimental work.

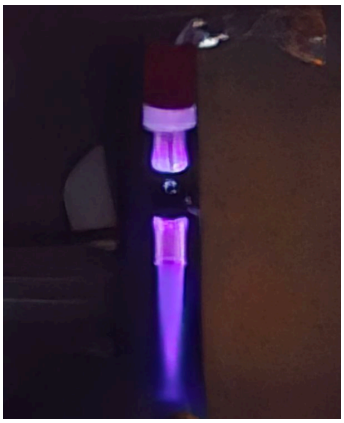


Figure 1: **An Argon plasma jet produced by a DBD plasma source.**

ACKNOWLEDGEMENTS

Acknowledging the support of the Australian Research Council (ARC) for funding this research.

Bibliography

[1] T. Kava, J. Evans, and I. D. Boyd, “Numerical Simulation of Electron-Beam Powered Plasma Fueled Engines,” in *AIAA Propulsion and Energy 2021 Forum*, VIRTUAL EVENT: American Institute of Aeronautics, Astronautics, Aug. 2021. doi: 10.2514/6.2021-3241.

Machine Learning Collision Models to Accelerate Direct Molecular Simulation of Rarefied Flows in Diatomic Gases

N. Daultry Ball[1,a)], J. Sirignano,[1] and J. MacArt[2]

[1]*Mathematical Institute, Woodstock Rd, Oxford, OX2 6GG, UK*
[2]*Fitzpatrick Hall of Engineering, 112 N Notre Dame Ave, Notre Dame, IN 46556, United States*

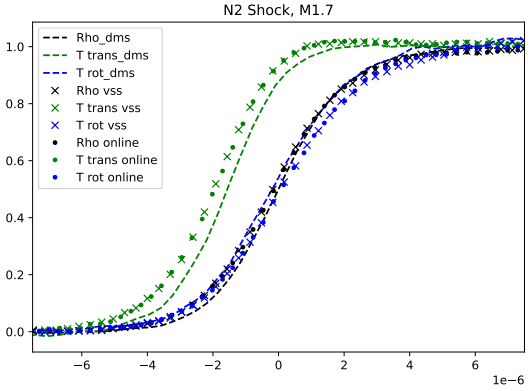
[a)]Corresponding author: nicholas.daultryball@maths.ox.ac.uk

We extend our previous work on machine learning collision models to accelerate simulations of rarefied flows [1] to the diatomic case, with results for one-dimensional normal shock waves in nitrogen. Our machine learning accelerated DMS method can now also be incorporated within SPARTA.

Direct Molecular Simulation (DMS) is a high fidelity method of simulating rarefied gases by incorporating numerical trajectory calculations into the Direct Simulation Monte Carlo (DSMC) algorithm. It can achieve accuracy comparable to Molecular Dynamics, but is substantially more computationally expensive than DSMC.

We accelerate DMS by replacing the computationally costly Classical Trajectory Calculations (CTC) with a machine learning model, optimised online during the simulation on a small dataset of CTC trajectories generated in situ during simulations. In the monatomic case, this involves learning a two dimensional function from the collision energy and impact parameter to the scattering angle. However, the diatomic case is significantly more complex due to the need to model the exchange of rotational energies between molecules. The trajectory calculation is also highly sensitive to the initial, randomly selected molecular orientations, so our machine learning surrogate takes the form of a Mixture Density Network which is able to learn the distribution of the scattering angle and post collision kinetic and rotational energies, given the pre-collision state. Replacing trajectory calculations with evaluation of the network, followed by sampling from the resulting distribution, results in significant computational speed up.

Initial results for a shock in Nitrogen are shown in Fig a), obtained by incorporating the DMS and online training algorithms within the SPARTA open source software package [2]. The shock profiles calculated with the ML-DMS method currently show comparable accuracy to those obtained with the VHS method. This initial proof of concept shows that the ML approach is able to give qualitatively good results. In particular the correct downstream equilibrium is reached, showing that the surrogate collision model is able to learn to respect detailed balance,a key physical property which must be respected by any model[3], without this being explicitly enforced.



Initial results for a shock in Nitrogen at Mach 1.7, comparing density and translational and vibrational temperature profiles between DMS, VHS DSMC and our online trained neural network model.

ACKNOWLEDGEMENTS

This work was supported by the EPSRC Centre for Doctoral Training in Mathematics of Random Systems: Analysis, Modelling and Simulation (EP/S023925/1), and by the U.S. Department of Defense, Office of Naval Research, under Award N00014-22-1-2441.

REFERENCES

[1] N. Daultry Ball, J. F. MacArt, J. Sirignano, *Journal of Computational Physics* **549**, 114601 (2026).
[2] S. J. P. et al., *Physics of Fluids* **31** (2019).
[3] A. L. Garcia, Dsmc: A statistical mechanics perspective, 2025, arXiv:2501.07785 [cond-mat.stat-mech]

Poiseuille coefficient for mixtures of rarefied gases: measurements and modelling

I. Graur[1,a)], F. Sharipov[2], E. Grigorov,[1], P. Perrier[1] and F. Topin[1]

[1]*Aix-Marseille Université, CNRS, IUSTI UMR 7343, 5 rue E. Fermi, 13453, Marseille, France*
[2]*Departamento de Física, Universidade Federal do Paraná, Curitiba, 81531-980, Brazil*

[a)]Corresponding author: irina.martin@univ-amu.fr

In many applications involving rarefied gas flows, it is more common to deal with gaseous mixtures rather than a single gas. However, both theoretical and experimental date on mixtures of rarefied gases are very poor. In the present work, a methodology for measuring the flow rate of a gaseous mixture through a long capillary based on the constant-volume technique is proposed. A theoretical modelling of such mixture flows was performed to justify the experimental method. Two mixtures, namely, He-Ar and He-Kr, were used in the experiments at various helium molar fractions ranging from 10 to 90 %. An analytical expression for the pressure variation over time in the inlet tanks, previously derived in Refs. [1, 2], is used here to extract the Poiseuille and velocity slip coefficients for the considered mixtures. These coefficients exhibit a non-monotonic dependence on the helium molar fraction. The experimental data for the dimensionless flow rate (Poiseuille coefficient) are compared with the previously obtained theoretical results based on the McCormack model [3]. The results are in agreement with each other within the experimental uncertainty. Moreover, using the proposed approach, the viscosity coefficient of the mixtures was also extracted, which was found in a good agreement with the values based on the *ab initio* calculations [4].

ACKNOWLEDGEMENTS

The study was supported by the ANR TEGTIC project number ANR-23-CE51-0055-01.

REFERENCES

[1] F. Sharipov, I. Graur, *Vacuum* **240**, 114585 (2025).
[2] E. Grigorov, F. Sharipov, P. Perrier, F. Topin, I. Graur, *Journal of Fluid Mechanics* **1025**, A13 (2025).
[3] F. Sharipov, D. Kalempa, *Phys. of Fluids* **17**, 127102 (2005).
[4] F. Sharipov, V. J. Benites, *Fluid Phase Equilibria* **498**, 23–32 (2019).

Towards Efficient Aerosol Injector Design for Generating Protein-Sized Nanoparticle Beams

S. K. Peravali[1,2,a)], J. He[2], A. K. Samanta,[2,3], P. Neumann,[5], J. Küpper,[2,3,4] and M. Breuer[1]

[1]*Professur für Strömungsmechaik, Helmut-Schmidt-Universität / Universität der Bundeswehr Hamburg, 22043 Hamburg, Germany*
[2]*Center for Free-Electron Laser Science CFEL, Deutsches Elektronen-Synchrotron DESY, 22603 Hamburg, Germany*
[3]*Center of Ultrafast Imaging, Universität Hamburg, 22761 Hamburg, Germany*
[4]*Department of Physics, Universität Hamburg, 22761 Hamburg, Germany*
[5]*Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany*

[a)]Corresponding author: peravals@hsu-hh.de

Protein-sized nanoparticles (< 20 nm) present a unique challenge for aerodynamic focusing in rarefied gas environments due to their extremely low inertia and high diffusivity. In this regime, Brownian motion and non-equilibrium gas–particle interactions dominate beam evolution, often leading to significant divergence and transmission losses. Despite their importance for single-particle diffractive imaging (SPI) experiments with X-ray free-electron lasers [1], the transport and focusing behavior of such small particles remains poorly understood. Experimental characterization is particularly challenging, as optical detection of sub-20 nm particles is difficult and often lacks sufficient sensitivity [2]. In addition to transport challenges, protein-sized particles require rapid cooling during aerosolization to preserve their native-like structure. Solvent evaporation in vacuum environments can induce dehydration and structural alteration, making thermodynamic control during injection a critical design constraint [3].

In the present study the design and analysis of a cryogenically cooled aerosol injector is presented which enables precise control of particle beam density while maintaining conditions favorable for structural preservation. Design optimization was guided by a multiscale simulation framework combining Computational Fluid Dynamics (CFD) and Direct Simulation Monte Carlo (DSMC) with particle tracking [4]. The approach captures continuum-to-rarefied gas transitions and resolves particle transport, focusing behavior, and cooling rates under realistic operating conditions. Parametric investigations demonstrate that cryogenic pre-cooling significantly suppresses Brownian diffusion by reducing thermal velocity spread and enhances focusing efficiency for protein-sized particles compared to conventional room-temperature injection. The results provide quantitative design guidelines for injector geometry and operating parameters aimed at generating dense, well-collimated beams of protein-scale nanoparticles, thereby improving experimental conditions for high-resolution SPI studies. Beyond injector optimization, the developed simulation framework offers fundamental insight into the dynamics of low-inertia nanoparticles in rarefied flows and establishes modeling tools specifically suited for protein-scale aerosol transport.

ACKNOWLEDGEMENTS

This work was supported by the HELMHOLTZ Data Science Graduate School for the Structure of Matter (DASHH, HIDSS-0002), by the Helmut-Schmidt University, University of the German Federal Armed Forces Hamburg, and by Deutsches Elektronen-Synchtrotron DESY, a member of the Helmholtz Association (HGF).

REFERENCES

[1] R. Neutze, R. Wouts, D. van der Spoel, E. Weckert, J. Hajdu, *Nature* **406**, 752–709 (2000).
[2] J. Bielecki, F. R. N. C. Maia, A. P. Mancuso, *Structural Dynamics* **7**, 040901 (2020).
[3] C. A. Orengo, A. E. Todd, J. M. Thornton, *Current Opinion in Structural Biology* **9**, 374–382 (1999).
[4] S. K. Peravali, A. K. Samanta, M. Amin, P. Neumann, J. Küpper, M. Breuer, *Physics of Fluids* **37**, 033380 (2025).

Abstract 234

Phase-based Microwave Shock Velocity Interferometry

Toby J. van den Herik[1,a)], Christopher M. James[1]

[1] *The University of Queensland, Centre for Hypersonics.*

[a)] Corresponding author: t.vandenherik@uq.edu.au

Knowledge of the trajectory of a ducted shock wave is important to understanding the quality of flow produced by an impulse facility. Facilities such as shock tunnels, shock tubes, and expansion tubes use, sometimes multiple, shock waves in the generation of their test flows as a mechanism to raise the state variables of the flow. If a shock wave's trajectory through a driven tube is not of constant velocity, then it follows that the post-shock state variables of the gas will be non-uniform in time and space and so too will the conditions of the test section. "Amplitude-based" microwave interferometry is a method used successfully to measure the displacement and velocity of shock and blast waves with resolution on the order of a diameter of the tube through which they travel – a good summary of such efforts is given by Straede et. al [1] where a peak it amplitude of a "Doppler signal" is related to a fixed distance traversed by the tracked shock wave. This approach relies upon the modulation of phase of an electromagnetic wave by shock wave position as depicted in Figure 1. This work will attempt to reconstruct the trajectory of a shock wave through the X2 expansion tube at far higher resolution using a phase-based approach akin to the piston tracking method applied by Kurosaka [2], though with significant efforts made to drastically reduce the phase-wobble effects that dominate uncertainty in velocity.

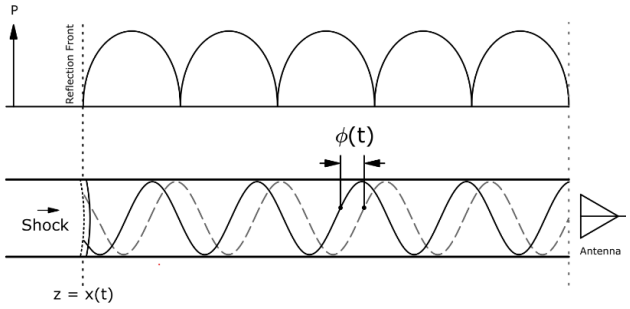


Figure 1 Dynamics of shock modulation of phase within a shock tube.

REFERENCES

[1] Henry G. Straede, Isaac Jenkinson, Toby J. van den Herik and Christopher M. James. "Implementation of Microwave Interferometry for Continuous Shock Speed Measurement in Shock and Expansion Tubes," AIAA 2024-2569. *AIAA SCITECH 2024 Forum*. January 2024.

[2] Kurosaka, Y. & Shimamura, K.. (2024). Microwave radar diagnostics of piston motion in a free-piston-driven expansion tube. Shock Waves. 34. 465-474. 10.1007/s00193-024-01194-1.

Abstract 235

Knudsen Force Acting on an Object with Curved Surface Placed near a Wall with Different Temperature

Kiyori Fujihara[1,a)] and Shigeru Yonemura[2]

[1] *Department of Mechanical Engineering, Graduate School of Engineering, Chubu University, 1200 Matsumoto-cho, Kasugai, Aichi 487-8501, Japan.*
[2] *Department of Mechanical Engineering, College of Engineering, Chubu University, 1200 Matsumoto-cho, Kasugai, Aichi 487-8501, Japan.*

[a)] Corresponding author: tm25009-0944@sti.chubu.ac.jp

When an object is immersed in a field where the gas temperature changes spatially on a length scale of several times of the mean free path of gas molecules, the molecules coming from regions of high temperature bring a large momentum to the surface of the object, whereas the molecules coming from regions of low temperature bring a smaller momentum. This imbalance causes a force on the surface of the object and its opposite reaction force is exerted on the gas. As a result, the gas flow is induced. The sum of the forces acting on the entire surface elements of the object is called Knudsen force [1]. Since the Knudsen force can be induced by using only heat as power source together with simple configuration of objects, the application of the Knudsen force to micro-devices is being investigated [2]. In this study, we focus on a Knudsen force acting on an object with curved surface placed near a wall whose temperature is different from that for the object. In particular, we conduct this study to deepen our understanding of the effect of the shape of object on the Knudsen force based on theoretical analysis and numerical simulations.

We consider a situation that a bow-shaped cold object is close to a hot wall. Figure 1 shows a pressure distribution and a flow field for the case where the arc-shaped surface of object is directed upward. Meanwhile, Fig. 2 shows those for the opposite case. The pressure p shown here is normalized by the spatially averaged pressure p_0 over the computational domain. In both cases, outward thermal edge flows are generated at both the edges of the object. Due to the pumping effect of the thermal edge flows, the pressure in the narrow region between the upper hot wall and the cold object is reduced. On the other hand, low pressure also appears over the bottom surface of the object in both cases. From these pressure distributions, it does not seem to generate a significant Knudsen force in any direction. However, the upward Knudsen force is exerted on the upward bow-shaped object and the downward Knudsen force is exerted on the downward bow-shaped object. The reason of this phenomenon will be discussed at the symposium.

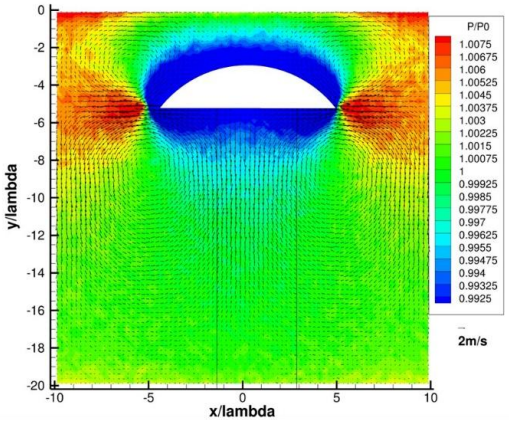


Fig.1 Pressure distribution and flow field in the case of the upward bow-shaped object.

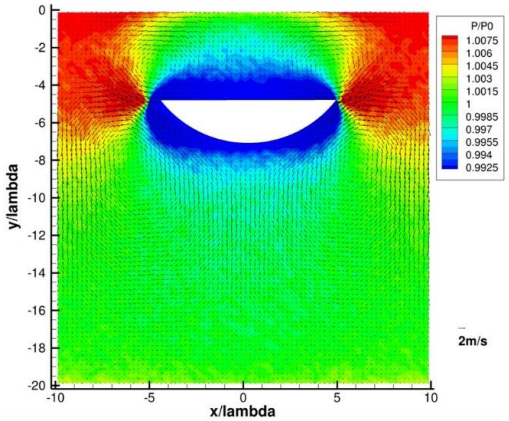


Fig.2 Pressure distribution and flow field in the case of the downward bow-shaped object.

REFERENCES

[1] Nabeth, J., Chigjullapalli, S., and Alexeenko, A., *Phys. Rev. E*, Vol. 83, No. 6 (2011), 066306.
[2] Strongrich, A. and Alexeenko, A., *Applied Physics Letters*, Vol.107, No. 12 (2015), 193508.

Experimental Observations of Plasma Wakes Created by Charged Bodies

C. A. Maldonado[1,a], M. S. Dunn[1], G. R. Wilson[1], and R. Ulrich[2]

[1] *Los Alamos National Laboratory, MS-D436, PO Box 1663, Los Alamos, NM 87545*

[a)] cmaldonado@lanl.gov

With refined gravity models, spacecraft drag has now become the largest source of error for orbital propagation of satellites operating in LEO [1, 2, 3]. These advancements have decreased uncertainties for elongated and non-compact satellite geometries; however, *a critical aspect of spacecraft drag that has never been experimentally quantified is charge induced ionospheric drag.* Spacecraft in LEO develop a negative charge due to an unequal collection of ambient ionospheric electrons and ions on exposed surfaces in addition to emitting photoelectrons due to ultraviolet photon bombardment. The accumulated charge generates an electric potential with respect to the ambient plasma. The negative charge on a LEO satellite creates an electrostatic potential called the spacecraft sheath that extends beyond the surface of the spacecraft. This electrostatic field impacts ions in three ways: (1) Ions are accelerated as they enter the spacecraft sheath and collide with spacecraft surfaces with greater energy than their unaffected neutral counterparts resulting in enhanced ion drag. (2) Ion trajectories are deviated as they enter the electrostatic field such that ions that would have otherwise passed by the spacecraft without impacting, are instead perturbed such that they collide with spacecraft surfaces. (3) Ions whose trajectories are perturbed but do not strike the spacecraft transfer momentum as they pass through the spacecraft sheath. Previous modeling efforts indicate that charge induced drag can increase overall spacecraft drag by an order of magnitude greater than from neutral drag alone [4]. The ability to accurately characterize and apply momentum transfer as a function of spacecraft charge will allow for an unprecedented improvement in orbital propagation and spacecraft traffic management. The ability to maneuver spacecraft using biased panels and geometries will allow for active orbital decay to de-orbit decommissioned spacecraft. This will also allow for propellant-less pointing maneuvers to enable longer mission lifetimes which are currently limited by the amount of fuel a spacecraft can carry. Initial experimental measurements of charge induced drag have been conducted using a LEO plasma emulator, shown in Figure 1. These initial measurements show changes in the wake structure due to applied negative and positive biases. Further experiments will be conducted to explore wake structures as a function of applied biases, both symmetric and asymmetric.

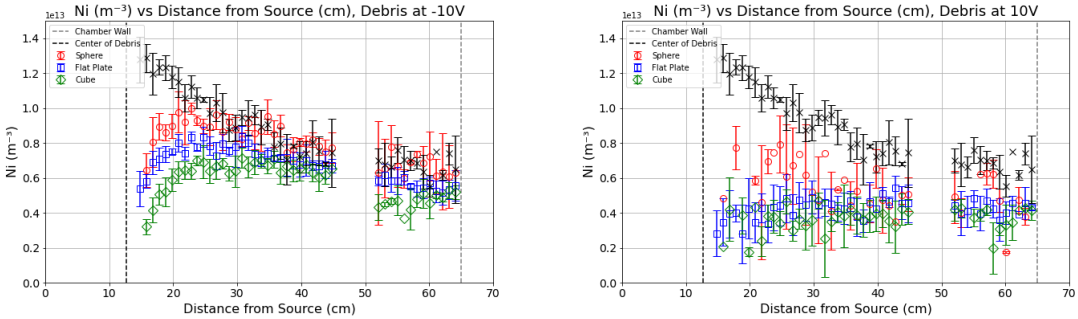


Figure 1. Experimental measurements of ion wake structures for (left) negatively biased (-10V), and (right) positively biased (+10V) simple geometries.

REFERENCES

[1] K. Moe and M. Moe, "Gas-surface interactions in low-Earth orbit," in *Proceedings of the 27th International Symposium on Rarefied Gas Dynamics*, Asilomar, CA, 2010.

[2] D. A. Vallado and D. Finkleman, "A critical assessment of satellite drag and atmospheric density modeling," in *AAS/AIAA Astrodynamics Specialist Conference*, Honolulu, HI, 2008, AIAA-2008-6442.

[3] C. M. Cox and F. G. Lemoine, "Precise Orbit Determination of the Low Altitude Spacecraft TRMM, GFZ-1, and EP/EUVE Using Improved Drag Models," in *Spaceflight Mechanics*, vol. 102, Advances in the Astronautical Sciences, 1999, pp. 1277-1296.

[4] C. J. Capon, B. Smith, M. Brown, R. Abay and R. R. Boyce, "Effect of ionospheric drag on atmospheric density estimation and orbit prediction," *Advances in Space Research,* vol. 63, pp. 2495-2505, 2019.

Abstract 237

TDLAS characterisation of magnetic field deformation within a hypersonic MHD flowfield

A. Lefevre[1,a)], D. E. Gildfind[1], T. Vanyai[1], T. J. McIntyre[1], J. Hendricks[1], T. Muramatsu[2], and K. Shimamura[2]

[1] *The University of Queensland, St. Lucia, Queensland 4072, Australia.*
[2] *Tokyo Metropolitan University, 6-6 Asahigaoka, Hino, Tokyo 191-0065, Japan.*

[a)] Corresponding author: a.lefevre@uq.edu.au

Magnetohydrodynamic (MHD) flow control concepts such as MHD aerobraking rely on strong coupling between ionised hypersonic flows and externally applied magnetic fields. Under flight-relevant conditions, the magnetic Reynolds number $Re_m = \mu_0 \sigma U L$ may exceed unity, causing the magnetic field to be advected and distorted by the plasma flow. This magnetic-field deformation can significantly alter the Lorentz force distribution and may reduce the effectiveness of MHD aerobraking concepts. Experimental measurements of magnetic-field advection in MHD controlled flows are therefore required to validate high-Re_m MHD models. Recently, Muramatsu et al. demonstrated a non-intrusive optical technique for magnetic-field measurements in hypersonic flows using tunable diode-laser absorption spectroscopy (TDLAS) combined with the Zeeman effect [1]. In experiments conducted in the HEK-X expansion tube, Zeeman splitting of the Ar I 794.8 nm absorption line was used to infer the path-averaged magnetic-field strength within the shock layer surrounding a magnetised test model. The present study applies this technique to investigate magnetic-field deformation in high-Re_m MHD flows, using the X2 expansion tube at the University of Queensland (typical setup illustrated in Fig. 1). New test flow conditions are developed in order to generate strongly pre-ionised argon flows to produce an MHD interaction zone with $Re_m > 1$. Under these conditions the magnetic field is expected to be convected along plasma streamlines. A cylindrical permanent magnet is used to generate the initial magnetic-field distribution, while a fibre-based TDLAS system probes the Ar I 794.8 nm transition to measure Zeeman-induced spectral splitting during the microsecond-scale test time. The resulting measurements aim to provide the first experimental observations of magnetic-field transport and deformation in hypersonic MHD flows at elevated magnetic Reynolds numbers.

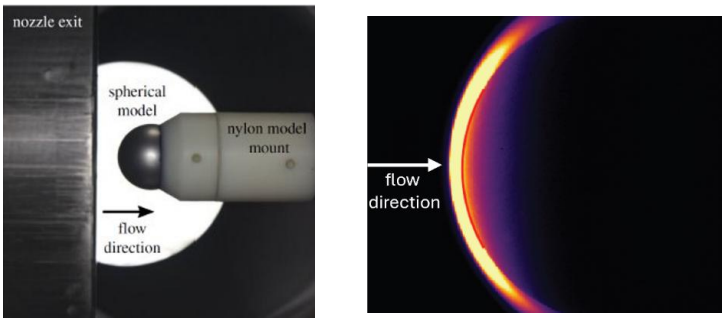


Fig. 1: Hypersonic flow around a high strength permanent magnet in X2, before (left picture) and during (right picture) experiment

ACKNOWLEDGEMENTS

The authors wish to thank the Australian Research Council for support and funding; the UQ High Performance Computing (HPC) Support Group for supercomputing support. This research was supported by the Australian Government through the Australian Research Council's Discovery Projects funding scheme (DP220101478 and DP250102748).

REFERENCES

[1] T., Muramatsu et al., *Characterization of Magnetic Field in Hypersonic Flow Using Tunable Diode-Laser Absorption Spectroscopy*, AIAA SciTech, 2026.

Abstract 238

The Aerodynamic and Acoustic Performance of a Bumblebee-Inspired Vehicle in the Martian Atmosphere

N. Widdup[1,a)], L. Wang[2], J. Young[1] and F. B. Tian[1]

[1]*School of Engineering and Technology, University of New South Wales, Canberra, ACT 2600, Australia*

[2] *Australian National University, Canberra, ACT 2601, Australia.*

[a)] Corresponding author: n.widdup@unswalumni.com

Martian exploration, particularly with the use of unmanned aerial vehicles (UAVs), has gained much traction in recent years. However flight on Mars is challenging due to the rarefied atmosphere, where the density is around ~1% of Earth's [1]. This subsequently results in a low Reynolds number environment for Martian UAVs. For this reason flapping wings are considered as a potential efficient design solution as birds and insects have been evolutionarily optimised for low Reynolds number flight [2]. However, the higher wing speeds required to generate lift, and the rarefied environment present unknown effects on the unsteady flow structures that flapping wings rely on for efficient lift generation, which this study investigates. In addition to considering the aerodynamic forces, this study also considers the near-field acoustic profiles for potential passive communication applications.

This study quantifies the effect of compressibility and rarefaction on the aerodynamics and aero-acoustics of a bumblebee configuration by means of numerical simulation. To decouple the effects of rarefaction and compressibility, the average wing tip Mach number (*Ma*) is varied from 0.6 to 1.4, and the Knudsen number (*Kn*) is varied from 0 to 0.05 with a second-order slip model implemented for $Kn \geq 0.01$ [3,4]. An in-house CFD solver is implemented for this research, which solves the 3D compressible Navier-Stokes equations and implements an immersed boundary method to accurately capture the fluid structure interaction [3,4]. A Taylor-series expansion of the equation of state is also implemented to ensure accuracy of wave propagation and allows for near-field acoustic analysis [3]. The numerical results show that rarefaction offers an improvement in the lift coefficient mainly attributed to a decrease in the viscous force, while the increase in Mach number results in lift reduction due to the pressure variations. The introduction of the slip boundary results in some minor changes in pressure forces due to a change in the formation and development of the vortex structures at the leading edge of the wing. Acoustic signatures are a function of *Ma* due to the generation, propagation and interaction of shock waves. Increasing *Kn* resulted in some minor changes in sound pressure level amplitudes, however the shape profile of the sound pressure level and the first and second fundamental frequencies remained unchanged from the no-slip $Kn = 0$ case.

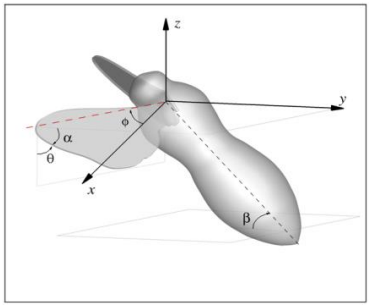


Fig. 1. Bumblebee configuration.

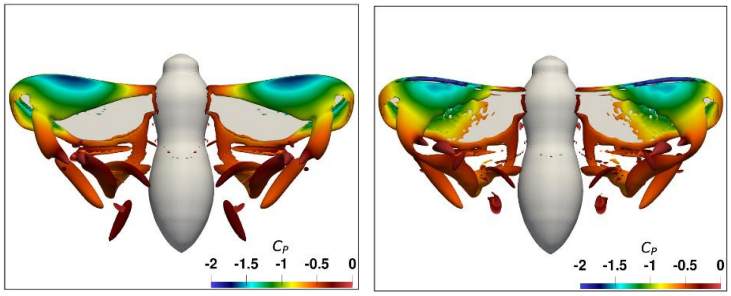


Fig. 2. Vortex structures in the mid-stoke for $Ma = 0.6$, $Kn = 0$ (left) and $Ma = 0.6$, $Kn = 0.5$ (right). Vortex structures are visualized by the Q-criterion ($Q = 2$) and coloured by the pressure coefficient.

REFERENCES

[1] Bézard, Hervé, et al. "Numerical and experimental aerodynamic investigation of a micro-UAV for flying on Mars." 76th Annual Forum & Technology Display. 2020.

[2] Ania, Asier, et al. "Flapping wing devices for mars exploration." Proceedings of the Canadian Engineering Education Association (CEEA) (2004).

[3] Widdup, Nathan, et al. "The aerodynamic and acoustic performance of a bumblebee-inspired micro-air vehicle in Martian atmosphere." Physics of Fluids 37.9 (2025).

[4] Wang, Li, John Young, and Fang-Bao Tian. "An immersed boundary method for the thermo–fluid–structure interaction in rarefied gas flows." Physics of Fluids 36.1 (2024).