AFRL-RV-PS-
TR-2023-0044

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TR-2023-0044

COMPUTATIONAL MODELING OF A TABLE-TOP SHOCK TUNNEL CONCEPT

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26 April 2023

Final Report

AIR FORCE RESEARCH LABORATORY
Space Vehicles Directorate
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AIR FORCE MATERIEL COMMAND
KIRTLAND AIR FORCE BASE, NM 87117-5776

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*
26-04-2023

2. REPORT TYPE
Final Report

3. DATES COVERED *(From - To)*
02 Jun 2020 – 15 Apr 2023

4. TITLE AND SUBTITLE
Computational Modeling of a Table-Top Shock Tunnel Concept

5a. CONTRACT NUMBER
FA9453-20-1-0012

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
C6601F

6. AUTHOR(S)
Thomas E. Schwartzentruber

5d. PROJECT NUMBER
1010

5e. TASK NUMBER
EF134671

5f. WORK UNIT NUMBER
V1L1

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Regents of the University of Minnesota
Office of Sponsored Projects Administration
200 Oak St. SE #224
Minneapolis, MN 55455-2009

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Air Force Research Laboratory
Space Vehicles Directorate
3550 Aberdeen Avenue SE
Kirtland AFB, NM 87117-5776

10. SPONSOR/MONITOR'S ACRONYM(S)
AFRL/RVBN

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
AFRL-RV-PS-TR-2023-0044

12. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited (AFRL-2023-02301 dtd 12 May 2023).

13. SUPPLEMENTARY NOTES

14. ABSTRACT

Hypersonic flight through the atmosphere generates extreme aerothermodynamic conditions. Specifically, a high-temperature shock layer is formed in front of the vehicle that can exceed 10,000 degrees Kelvin. Recently, a novel experimental approach for measuring shock layer physics has been designed and constructed; called the Table-Top Shock Tunnel (TTST). The basic idea is that a pulsed molecular beam, when targeted at a small blunt object, can generate a hypersonic shock layer that exhibits relevant gas-phase dissociation and gas-surface reaction physics in a small lab setting. This project involves computational research to characterize the flow conditions in the TTST facility and then validate gas-phase and gas-surface reaction chemistry models with the new data.

15. SUBJECT TERMS
hypersonic flow, numerical simulation, chemistry, ablation

16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT**	**18. NUMBER OF PAGES**	**19a. NAME OF RESPONSIBLE PERSON**
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**			Capt. Jason G. Seik
Unclassified	Unclassified	Unclassified	Unlimited	24	**19b. TELEPHONE NUMBER** *(include area code),*

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. 239.18

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ACKNOWLEDGMENTS

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1. SUMMARY

Hypersonic flight through the atmosphere generates extreme aerothermodynamic conditions. Specifically, a high-temperature shock layer is formed in front of the vehicle that can exceed 10,000 degrees Kelvin. Experimental measurements of such extreme conditions are challenging and flight conditions cannot be truly reproduced. Computational modeling, now based on quantum chemistry, has outpaced the capability to validate experimentally. For this reason, new optical diagnostic data measured under relevant hypersonic flow conditions is badly needed. Recently, a novel experimental approach for measuring shock layer physics has been designed and constructed; called the Table-Top Shock Tunnel (TTST). The basic idea is that a pulsed molecular beam, when targeted at a small blunt object, can generate a hypersonic shock layer that exhibits relevant gas-phase dissociation and gas-surface reaction physics in a small lab setting. This project involves computational research to characterize the flow conditions in the TTST facility and then validate gas-phase and gas-surface reaction chemistry models with the new data. The development of hypersonic flight models and technology is currently a priority of the US Department of Defense. The public purpose of the proposed computational research is to support optimization of the new TTST facility, characterization of the flow environment, and validate new chemical reaction models. The success of this laboratory-scale facility provides an exciting new capability for the high-speed flow community and high-energy particle effects community.

2. INTRODUCTION

Hypersonic flight through an atmosphere generates a thin, high-temperature, shock layer that surrounds the vehicle surface, typically a heat-shield material. Within this shock layer, the gas is in a state of strong thermochemical nonequilibrium. The internal energy of the gas (rotational and vibrational energy) quickly increases and ultimately leads to dissociation of molecular species into atomic species. These reactive atomic species (O and N) diffuse through the boundary layer and react with the heat-shield surface. If the heat shield is ablative, reaction products are transported back into the flow, which in turn affects the chemical state of the boundary layer. In this manner, the dissociation process within the shock layer (the supply of reactive atomic species) has a first-order effect on degradation of the vehicle heat shield, which is one of the major challenges associated with hypersonic flight and vehicle design.

Current experimental measurements of the shock layer are incredibly difficult and expensive to perform. Ground-based experiments cannot reproduce a wide range of flight conditions and vehicle configurations. Therefore, accurate and predictive models are required for use in computational fluid dynamics (CFD) simulations. The most widely used vibrational energy model is the Millikan-White model [1], and the most widely used dissociation model is the Park TTv model [2]. Both of these models are empirical and based on relatively few experimental data sets (examples for nitrogen are seen in Refs. [3]-[5]). Their accuracy outside of the limited experimental conditions is uncertain, and this uncertainty directly affects all other coupled processes.

In order to reduce this uncertainty, a significant amount of research has been performed using computational chemistry [6-20]. These first-principles, predictive simulations and models have been shown to reproduce the limited experimental results [1,3-5] used to construct the empirical Millikan-White and Park TTv models. However, the first-principles calculations differ significantly from these empirical models for other hypersonic conditions where no experimental data exist [8,10,11,12,16]. Furthermore, new gas-surface reaction models have been recently developed based on molecular beam experiments [21-23], that involve single collision interactions between high energy atoms/molecules and pre-heated material samples. These new physics-based models need to be validated under conditions relevant to hypersonic boundary layers. In order to validate both gas-phase and gas-surface reaction models, new optical diagnostic data measured under relevant hypersonic flow conditions is badly needed. Such experiments are extremely challenging/expensive and no such data sets, sufficient to validate new models, have been generated to date.

Why are optical measurements so difficult in hypersonic flows? The main problem is that true hypersonic conditions can only be sustained for short test times (microseconds to milliseconds). Collecting optical diagnostic data during such short timescales in a high-temperature gas is extremely difficult (low signal to noise). Furthermore, high-enthalpy facilities tend to be large facilities where only a few tests can be performed per day and precise repeatability between tests is difficult. Such facilities exist at CUBRC [24], the University of Queensland [25], the NASA Ames EAST facility [26], Stanford University [5], and the Caltech T5 tunnel. Alternatively, lower-enthalpy facilities have longer test times, and therefore optical measurements can be made more easily. However, the relevant thermochemical nonequilibrium processes in the shock layer are no longer present. Such facilities include those at the University of Canberra [27], the Caltech expansion tunnel (formerly located at the University of Illinois) [28], and Ohio State University [29].

In 2020-2021, through support from AFRL and a DURIP award, a novel experimental facility, called the Table-Top Shock Tunnel (TTST) has been constructed at the University of Colorado Boulder by Prof. Tim Minton’s research group, with numerical simulation support from PI Schwartzentruber’s group. The TTST facility is designed to enable high quality measurements of nonequilibrium gas-phase chemistry and gas-surface chemistry under relevant hypersonic conditions in a laboratory setup. The basic idea is that a pulsed molecular beam, when targeted at a small blunt object, can generate a hypersonic shock layer that exhibits relevant dissociation physics. Unlike large shock-tunnel facilities, the beam, and therefore the shock layer, can be generated (pulsed) 2-5 times per second for hours with repeatable conditions. Such test frequency and repeatability would enable existing optical diagnostic techniques to measure thermochemical quantities with unprecedented accuracy and precision at a fraction of the cost compared to existing shock tunnel facilities. In addition to studying shock layer dissociation, this approach would also enable optical diagnostic measurements of hypersonic flow over ablative heat shield materials.

Research Goals: This project involves computational research to support further design of the TTST facility, to guide the choice of optimal operating conditions and test article geometry, to characterize the flow conditions and interpret the experimental measurements, and to validate the new gas-phase and gas-surface chemistry models. If successful, the TTST laboratory-scale facility would provide an exciting new capability for the high-speed flow community and high-energy particle effects community.

Due to the rarefied nature of the TTST flow, the simulations are performed using the direct simulation Monte Carlo (DSMC) method. The DSMC approach is described along with the experimental setup in Section 3. DSMC simulation results of Kapton material in the TTST are described in Section 4.1, where the simulations help characterize the overall beam flux in the facility. With the beam flux accurately characterized, DSMC results for the ablation of a carbon sample in the TTST are discussed in Section 4.2, along with comparison to experimental data. Finally, conclusions of this project are summarized in Section 5.

3. METHODS, ASSUMPTIONS, AND PROCEDURES

The TTST apparatus, exploits existing technology in hyperthermal beams and laser-based diagnostics to build a low-cost shock tunnel, which, despite its small size, can be used for rapid acquisition of high-fidelity data on shock-layer chemistry and gas-surface chemistry that will provide definitive validation of emerging dissociation and ablation models. This facility fits in a common laboratory space, and the vacuum chamber (including the hypersonic beam, target, and beam diagnostics) occupies a footprint no larger than a typical laser table. The hypersonic beam is based on the laser-detonation source that has been used by Prof. Tim Minton's group at Montana State University (MSU) for more than 25 years in studies of hyperthermal gas-phase and gas-surface scattering dynamics. This beam can create reproducible and intense pulses of gas with nominal velocities of 4-9 km/s at repetition rates of 2-5 Hz.

The novelty of the TTST facility is threefold. (1) A well characterized gas or gas mixture (in terms of velocity distribution, mole ratio, and chemical state) can be directed at a target. (2) The high repetition rate and reproducibility of hypersonic pulses of sufficient intensity to form a shock above a target allows for high quality spectroscopic data to be obtained from standard diagnostic tools, such as coherent anti-Stokes Raman spectroscopy (CARS) or, possibly, laser induced fluorescence (LIF). (3) The target may be ablating or non-ablating; in the case of an ablating material, the sample may be heated to high temperatures, allowing for studies of the boundary layer above an ablating material to be investigated as well as studies of the ablated surface. This experimental setup is not appropriate to study fluid dynamic phenomena such as high Reynolds number flow (transition and turbulence), shock-boundary layer interactions, separated flow, and cannot exactly reproduce free-stream flight conditions. The point is, nevertheless, that no ground-based facility can capture all flight-relevant processes and provide a feasible means for optical measurements. The TTST concept focuses specifically on producing much-needed data for nonequilibrium dissociation and gas-surface interactions. It is this focus that will enable the TTST to obtain high-quality optical diagnostic data for relevant conditions that no other existing facility can.

The heart of the TTST is a laser-detonation hypersonic beam source, adapted from a source that has been operated for more than two decades in the Minton lab [30-40]. A schematic diagram of the source is seen in Fig. 1. A pulsed valve is used to inject gas

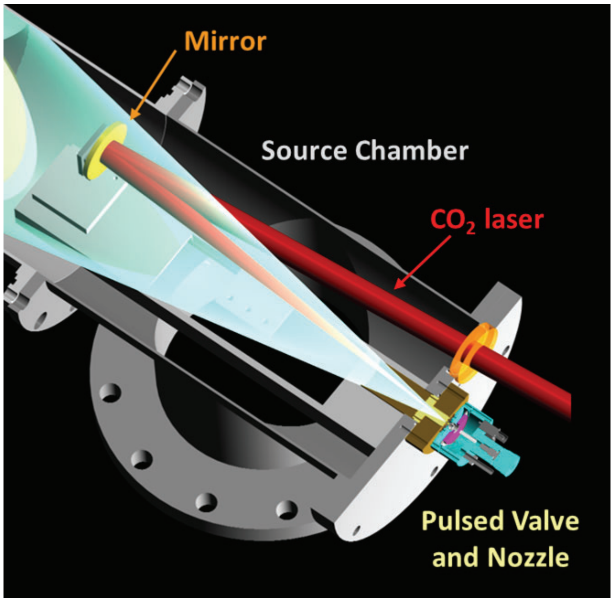


Figure 1. Laser-detonation hypersonic beam source

at high pressure (~550 psi) into the small end of a conical nozzle. After the gas expands into the nozzle, a 7 Joule per pulse CO_2 laser is fired, and the light is focused down into the nozzle where it induces a breakdown and heats the resulting plasma to more than 40,000 K. The detonation wave that is produced dissociates and accelerates the gas, and a neutral pulse emerges from the nozzle, containing partially dissociated gas, with the extent of dissociation depending on various operating parameters of the source. The pulse nominal velocity can be varied from about 3 to 9 km s^{-1}. Beams have so far been produced with precursor gases, O_2, N_2, Ar, CO_2, and N_2O. Mixtures of these gases may also be used, and one can imagine additional precursor gases. The hypersonic beam pulse is typically characterized by a mass spectrometer, which allows the species in the beam to be identified and their velocity distributions and mole fractions to be determined. The species are generally in their ground electronic states [41,42]. The hypersonic beam will be directed at a target surface that is placed in the path of the beam at various distances from the nozzle. This target may be ablating or non-ablating and may be temperature controlled from room temperature to >2000 K. The target may also be instrumented with sensors to measure heat flux, pressure, and shear stress.

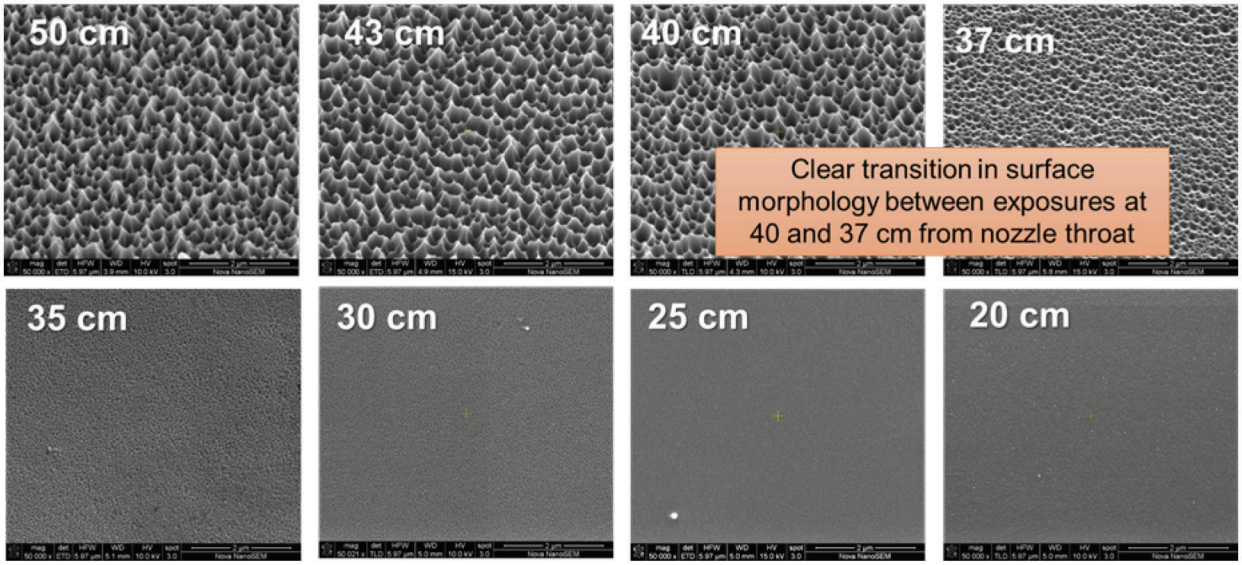
Due to the rarefied nature of the TTST flowfield, the direct simulation Monte Carlo (DSMC) method is used [43,44]. The DSMC method simulates the Boltzmann equation and is therefore accurate over entire range from free-molecular flow to continuum flow. The current TTST operating conditions lie in the transitional regime between free-molecular and continuum, and the near-surface conditions enter into the continuum regime. This results in DSMC simulations that are computationally demanding, but clearly feasible with current parallel computing power. We have used the Molecular Gas Dynamics Simulator (MGDS) DSMC code [45] developed at the University of Minnesota to simulate the TTST flowfields discussed in this report. We have used the Variable Hard Sphere (VHS) model for collisional cross sections, a constant collision number for rotational relaxation and Millikan and White vibrational relaxation times.

4. RESULTS AND DISCUSSION

4.1 Characterization of Beam Flux via Kapton Surface Erosion

Although the beam properties can be precisely measured by the mass spectrometer, such as the species mole fractions and the velocity distribution function, the overall flux in the beam cannot be easily measured. The beam flux must be characterized in order to perform matching numerical simulations, to interpret the TTST measurements, and ultimately validate new chemistry models. This section describes a joint computational/experimental campaign that uses the well-known erosion rate of Kapton to characterize the beam flux in the TTST.

A series of experiments were performed in the TTST facility where Kapton samples were exposed to a mixed O/O2 beam at increasingly large distances from the nozzle exit and the surface roughness and mass loss of each sample were measured. Scanning electron microscopy (SEM) images of each sample in Fig. 2 show a drastic change in surface morphology between the samples exposed at a distance of 40 cm and 35 cm from the nozzle. Figure 2 shows that for exposure distances larger than 35 cm the surface erosion of the Kapton samples start to result in sharp peaks and valleys that are not visible for lower distances. This is thought to be caused by the formation of a shock wave in front of the sample. High beam flux (short distance) is expected to result in significant compression and the formation of a shock, whereas lower flux (long distance) is expected to be too rarefied to form a highly collisional post shock state. By performing DSMC simulations with specific beam flux estimates and comparing the results to the experimental measurements, the actual beam flux in the facility can be determined.



Clear transition in surface morphology between exposures at 40 and 37 cm from nozzle throat

Figure 2. SEM images of Kapton samples for various exposure distances

For the DSMC calculations, the inflow conditions were kept constant in time, and each simulation was iterated in time until it reached steady state, after which results were sampled. Although the TTST is a pulsed beam, each simulation reached steady state in approximately the same time as one beam pulse, and the surface flux sampled from the steady state simulations adequately represents the experiment. The simulation conditions are shown in Table 1 and the simulation domain is pictured in Fig. 3.

The inflow conditions for simulations 1-8 were chosen based on measurements of the beam's composition, velocity distributions of its components, and estimates of the O atom flux based on the exposure at 40 cm distance and a commonly used Kapton erosion relation. The domain size was kept the same across simulations 1-8, so to simulate exposure at different distances from the nozzle, the inflow densities were scaled by r^{-2} with the distance from 40 cm. The beamwise velocities of the different species were sampled from gaussian distributions fit to the measured velocity distributions and the perpendicular velocities were sampled from Boltzmann distributions at 10 degrees K. The sample was broken up into three regions marked Center, Middle, and Edge as shown in Fig. 4 to study the velocity and impact angle distributions of particles at different radial distances on the sample face.

As expected, when the simulated beam flux is higher, corresponding to short distances between the nozzle and Kapton sample, significant gas compression is observed in front of the sample. Whereas, when the simulated flux is lower, corresponding to larger distances between the nozzle and Kapton sample, there is no distinct shock layer region. In order to analyze the results in a more quantitative manner, the DSMC simulations record all atomic oxygen (AO) impacts on the sample surface; the number of impacts, the velocity of the AO atoms upon impact, and the angle of impact are recorded in each of the three radial regions shown in Fig. 4.

Figure 5 shows two dimensional distributions of speed and impact angle for AO that impacts the sample surface in the simulation. The y axis represents the oxygen atoms' speed and the x-axis represents the angle their velocity makes with the inverse surface normal of the surface element they impact. Figure 5 shows that as the inflow density is lowered, more of the distributions' volume is at low angles and high velocities; specifically the maximum values seen in the upper left corner of the plots. The reason for this is that as the exposure distance is increased (lower beam density at the sample distance) the shock wave becomes increasingly diffuse, and incoming AO is less likely to undergo gas phase collisions before it impacts the sample surface. Figure 5 shows that as the exposure distance is increased (inflow density decreased), the surface AO flux is increasingly dominated by atoms that strike the surface unimpeded; speed near 8000 m/s and impact angle near 0 degrees.

Table 1. DSMC simulation conditions for comparison with experimental measurements

#	Representative Distance / Condition	Freestream O Atom Flux (Molecules m^{-2} s^{-1})	Composition	ρ_∞ (kg m^{-3})	Velocity Sampling
1	20 cm	4.76 x10^{25}	χ_O = 0.724 χ_{O_2} = 0.256	4.91 x10^{-5}	V_X: Beam Distributions V_Y and V_Z : Boltzmann @ 10 K
2	25 cm	1.19 x10^{25}		3.14 x10^{-5}	
3	30 cm	4.64 x10^{24}		2.18 x10^{-5}	
4	35 cm	2.61 x10^{24}		1.60 x10^{-5}	
5	40 cm	2.00 x10^{24}		1.23 x10^{-5}	
6	45 cm	1.58 x10^{24}		9.70 x10^{-6}	
7	50 cm	1.01 x10^{24}		7.86 x10^{-6}	
8	65 cm	7.57 x10^{23}		4.65 x10^{-6}	

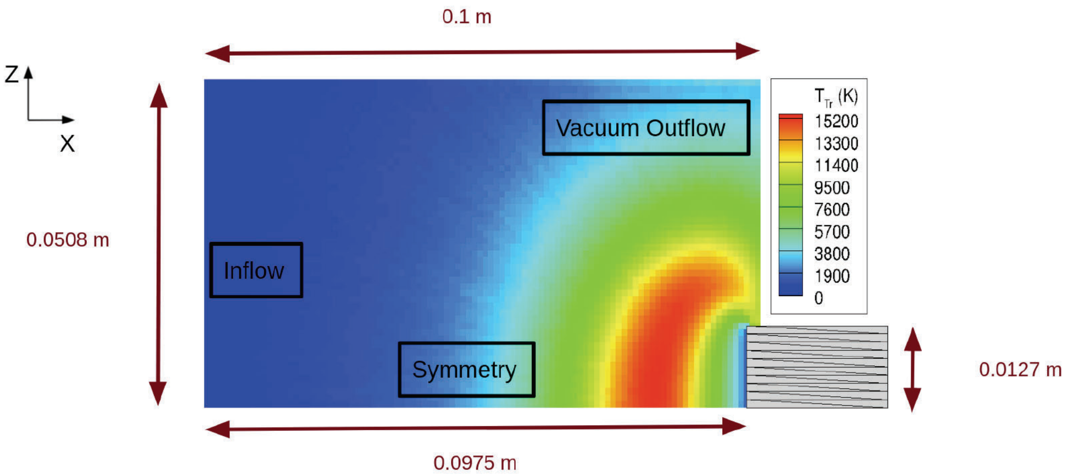


Figure 3. DSMC simulation domain and boundary conditions, with an example flow field solution

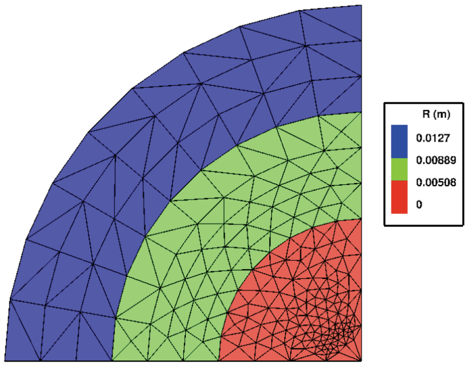


Figure 4. Radial zones on the Kapton sample used to study O atom impacts in the DSMC calculations

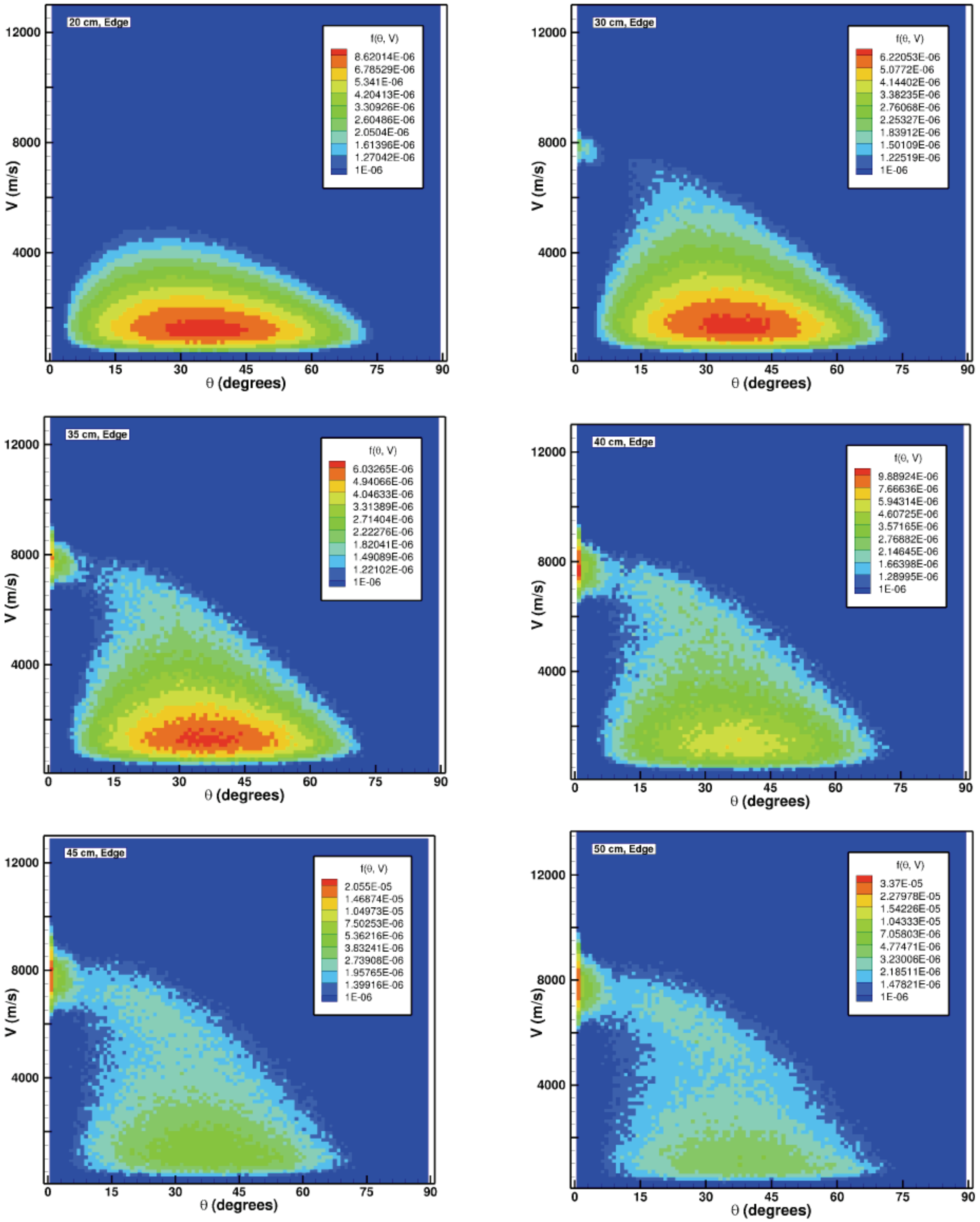


Figure 5: AO impact results from DSMC simulations corresponding to various nozzle-to-sample distances. *The probability distribution (f) of speed and angle is plotted for all AO impacts on the Kapton sample*

The trends in the DSMC results for surface flux are consistent with those observed in the beam exposure experiments shown in Fig. 2. At small exposure distances, SEM images of the exposed samples show that the surface is smooth. As the exposure distance increases, the surface of the sample starts to show sharp needle-like peaks with deep valleys in between them. This effect starts to become apparent between the exposure distances of 35 cm and 40 cm, which coincides with the DSMC simulations where the distribution of impacting O atoms starts to become dominated by particles with small deflection angles and high speeds. We conclude that the surface morphology effect seen in the experiments can explained by the fact that at closer distances the shock layer in front of the sample is stronger and incoming particles are more likely to be scattered by gas phase collisions before striking the sample face. These gas phase collisions cause the incoming oxygen atoms that erode the Kapton surface to have speeds much smaller than the inflow condition, and a large range of deflection angles. At lower density conditions the shock is weaker, and increasingly more O atoms strike the surface unimpeded. This explains the surface morphology effect seen in the experiment. A microscale model for the erosion of Kapton by atomic oxygen would allow more detailed studies of the surface morphology effect, but the current simulations explain the experimental trends well.

The overall conclusion is that, given the close agreement between DSMC and experiment, the beam flux used in the DSMC simulations (Table 1) accurately represents the beam flux in the experiments. Note that other DSMC calculations were performed with other beam flux values, but the closest match between simulation and experiment was found for the flux versus distance values in Table 1. This study of Kapton erosion has therefore provided a good estimate for the actual beam flux in the TTST facility. With the beam flux characterized, predictive simulations of TTST experiments can now proceed with greater accuracy.

4.2 Preliminary Validation of a New Carbon Ablation Model

While the original project proposal described further DSMC simulations to possibly improve the nozzle of the TTST, and simulations aimed at validating the gas-phase chemistry models, the focus of the simulations switched to ablation physics due to the experimental schedule. The TTST facility was augmented with the capability to heat carbon samples to high temperature while exposed to the TTST flow. An experimental campaign was carried out for an oxygen beam impacting a Vitreous Carbon (VC) sample heated to a wide range of temperatures and recession of the sample was measured. This was an exciting advancement given the importance of ablation in the hypersonics community and the recent development of a new ablation model from the Schwartzentruber and Minton groups. As a result, the project focused on validating the new carbon ablation model with this new, unique, experimental data set from the TTST facility.

Material samples of various types may be mounted in the TTST chamber on custom holders and placed in different locations with respect to the nozzle for exposure to the hypersonic beam. For the exposures of VC reported here, samples of 25 mm long × 7 mm wide × 1 mm thick were heated resistively by passing current through the sample, which was mounted between two water-cooled copper electrodes (see Fig. 6). Alumina plates were used on each side of the sample to create a stronger and more uniform shock layer above the plane of the sample than would be formed in the absence of the plates. The sample was placed at various distances from the nozzle throat and held at a constant temperature for each exposure to the hypersonic beam. The sample was offset slightly from the beam axis, because the central portion of the beam was allowed to pass through two apertures to a mass spectrometer for characterization of the free stream flow. Nevertheless, the sample surface was always perpendicular to the streamlines of the beam.

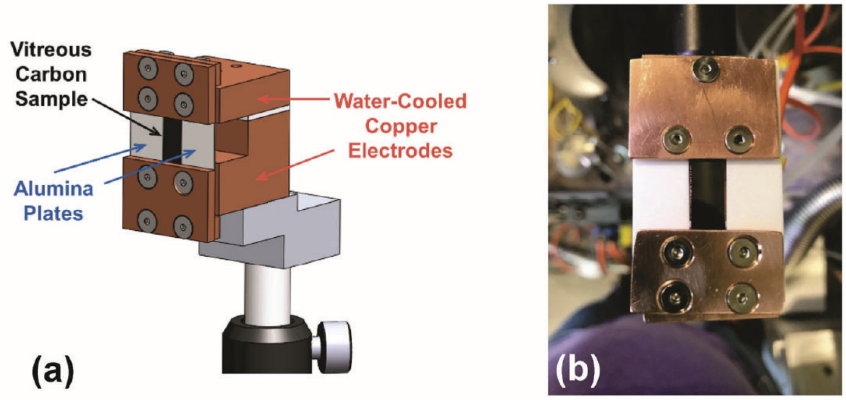


Figure 6: Schematic (a) and image (b) of the Vitreous Carbon sample and the heated sample mount configuration

Matching DSMC simulations were performed, using the beam flux characterized in the first phase of the project; summarized in Table 1. Example solutions are shown in Fig. 7. DSMC results (Fig. 7a) show that the TTST flow is expected to produce a diffuse shock layer in front of the sample mount, with translational temperatures exceeding 20,000 K behind the shock and cooling to the controlled VC surface temperature. As seen in Fig. 7b, the near-surface pressure, predicted by DSMC, is 50 Pa. While this pressure is far below the surface pressure expected during typical hypersonic flight (20-40 km altitude), it is orders-of-magnitude greater than the pressure in a surface-scattering molecular beam experiment, in which there are no gas-phase collisions.

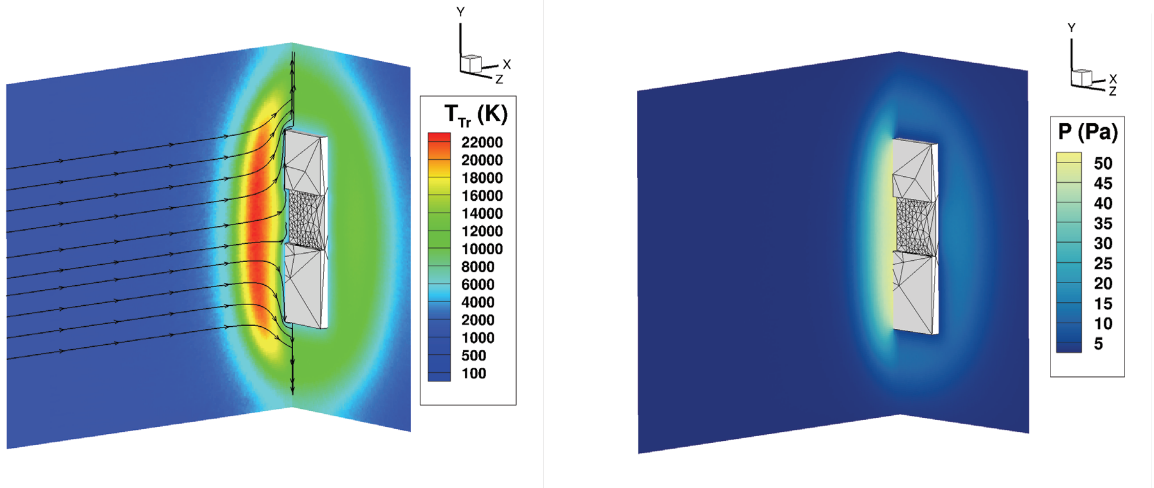


Figure 7: Example DSMC results for TTST flow over the VC sample and mount; translational temperature (left) and pressure (right)

In order to simulate carbon ablation, the new Air Carbon Ablation (ACA) model [46], developed for CFD simulations, was adapted and implemented into the MGDS DSMC code. This required considerable effort, not detailed in this report for brevity. To summarize, the ACA model includes surface coverage dependence (and therefore pressure dependence) by introducing the coverage (or availability) of various surface sites explicitly in the model. Tracking surface coverage in DSMC is not trivial due to statistical scatter inherent in every DSMC simulation. The clear first-step was to assume a fixed surface pressure and to evaluate the model at that pressure. This was done for various pressures. Since the near-surface pressure is seen to be very close to 50 Pa (Fig. 7), the model was evaluated at this pressure. In addition, the model was evaluated at the molecular beam surface-scattering pressure ("MB Flux"), and a very high pressure of 5400 Pa that is representative of large-scale inductively coupled plasma (ICP) wind tunnel tests. As a result, the ACA model now has only a temperature dependence, but a different temperature dependence for different pressures. These model results are shown in Fig. 8a. The key point is that the ACA model was fit to experimental data only at the "MB Flux" pressure condition (free-molecular flow and near-vacuum conditions), and that the trends at higher pressure are purely model predictions.

The TTST recession data is shown in Fig. 8b. Clearly the recession rate increases rapidly with increasing temperature. However, at a temperature near 1550 K, the recession rate begins to level-off and even decline as temperature is increased further. This is precisely the trend seen with the ACA model evaluated at the TTST relevant pressure (50 Pa line in Fig. 8a). In contrast, the model predictions at both lower and higher pressures do not follow the same trend as the TTST experiments. This is the strongest experimental evidence to-date that the temperature and pressure dependence captured by the ACA model is accurate. It should be noted that while the trends are comparable between DSMC and experiment, the absolute values are not directly comparable yet. This requires making the "recession" post-processed from the DSMC simulations to be consistent with the recession measured in the experiment. This work is ongoing.

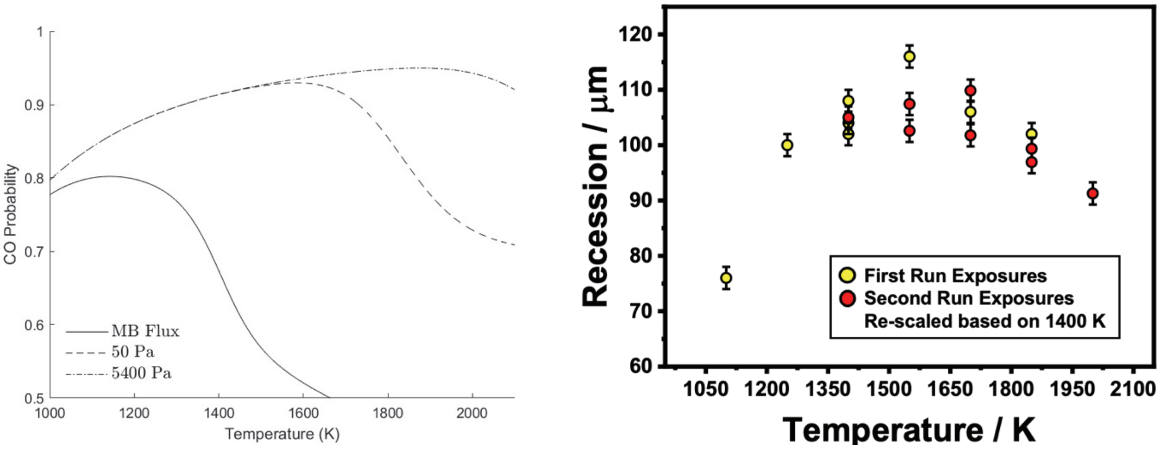


Figure 8: (a) ACA ablation model trends for reaction probability at three different pressures. (b) TTST experimental results for recession rate trend with temperature, where the near-surface pressure is estimated to be approximately 50 Pa (see Fig. 7b)

5. CONCLUSIONS

By performing DSMC simulations of the TTST facility and by comparing with experimental measurements, we were able to successfully characterize the overall beam flux in the TTST facility – a main goal of the project. Specifically, by varying the beam flux in the simulations we were able to match experimental observations of Kapton erosion for a specific value of the simulated beam flux. Using this beam flux in the DSMC simulations, we were able to match the Kapton sample location where a transition from free-molecular flow to highly collision flow (the formation of a diffuse shock wave) occurred experimentally. As a result, the overall beam flux in the TTST facility has been characterized, and this beam flux value now completes knowledge of the freestream flow conditions in the TTST. Furthermore, indirect evidence of shock-wave formation has been established, given the dramatic change in Kapton surface morphology observed.

The success of the Kapton erosion study enabled research to advance directly to study the ablation of pre-heated carbon samples. The new Air Carbon Ablation (ACA) model, developed for CFD simulations, was successfully implemented in the MGDS DSMC code. Preliminary simulations of the TTST flow over the 3D carbon sample and sample holder were performed. The surface pressure was determined to be approximately 50 Pa; much lower than flight conditions, yet orders of magnitude higher than the molecular beam surface-scattering conditions that the ACA model was constructed with. Using the ACA model at this pressure (50 Pa) the trend in reaction probability with temperature matches the trend observed in the new TTST carbon ablation experiments remarkably well. Two of the most important (and novel) aspects of the ACA model include the non-Arrhenius trend of the reaction probability with temperature and that the model naturally includes pressure dependence. Obtaining experimental data to validate these model predictions is currently not possible in large plasma wind tunnel testing. The TTST experimental data combined with the DSMC simulations performed under this project provide the best validation of the ACA model yet.

Further details for both the Kapton and Vitreous Carbon campaigns can be found in two recent AIAA Conference papers [47,48].

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