

# 10<sup>th</sup> Ablation Workshop

September 17-18, 2018

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Meyers et al., 2018

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## Abstracts of the 10<sup>th</sup> Ablation Workshop

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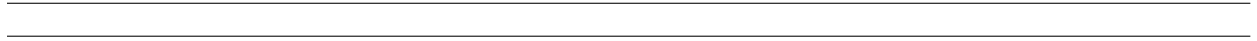




## Overview and welcome

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## Ablation Workshop: 10 Years of History

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## **Mars Sample Return: Grand Challenge for EDL**

Ethiraj Venkatapathy

An abstract for the 10<sup>th</sup> Annual Ablation Workshop

A year ago, I gave a talk in anticipation of a Mars Sample Return effort at the 9<sup>th</sup> Ablation Workshop. Since then a lot has happened.

“April of this year, after a year of study phase, NASA and ESA signed [Statement of Intent \(SOI\)](#) to jointly develop a Mars Sample Return plan to be submitted to their respective authorities by the end of 2019. This signing is historic, as it signals the desire, the readiness, and the willingness to work together to execute this inspiring mission, we all have the opportunity to tackle this grand challenge. We have the scientific and engineering maturity to identify the critical technologies ready to be applied, and with discipline this campaign can be executed affordably,” Jim Watzin, Mars Program Executive, NASA. NASA Centers with JPL leading the charge is in the midst of a pre-formulation phase for executing a Mars Sample Return before the end of next decade.

The proposed talk builds on the previous year talk. In light of the agreement between NASA and ESA, NASA has assumed the responsibilities for developing the earth entry vehicle (EEV) that will fly along with a European Spacecraft and return with the sample from Mars. EEV will be deployed for entry into earth. The EEV design, development, testing and certification have to result in a highly reliable sample return system. The entire architecture has to be demonstrated to meet the planetary protection requirement. NASA is considering two distinctly different earth entry vehicle architectures and with each choice, many different ablative TPS candidates. As a result of the NASA-ESA on-going studies, some of the key entry conditions and design requirements are better understood today and more are being scoped out.

The heat-shield ablative TPS choice need to be done with a good understanding as it plays a very significant role in determining the robustness of the EEV. Knowledge about how materials and system perform, and how the features could become flaws and how flaws lead to failure, etc. need to be clearly understood and the knowledge then need to be used to down select the TPS.

This proposed talk will provide greater insight into the progress being made and the challenges that need to be tackled.

## **TPS Architectures and the Influence of Material and Architecture on Failure Mode Evolution**

Mairead Stackpoole

An abstract for the 10<sup>th</sup> Annual Ablation Workshop

A primary focus of the Entry Systems and Technology Division at NASA Ames is design, development, qualification and certification of Thermal Protection Systems for current NASA missions. Another primary focus is the development of new thermal protection systems for upcoming missions that address shortfalls in the existing suite of TPS. Examples of such shortfalls include performance at higher capability and reduction in mass. NASA is also investing in TPS sustainability ensuring the long term availability of TPS solutions for future missions. The specific TPS selection, for a given mission, depends on a number of parameters including the missions risk posture. For all missions the goal for TPS is efficient and reliable performance and to achieve these goals an understanding of the materials (composition and architecture) is required for proper design and use of the chosen TPS. Analytic tools are used to inform on a material (systems) response to a given environment and the response itself depends on the materials properties which are driven by its composition and architecture. This presentation will review the different generic ablative TPS architectures and anticipated corresponding failure modes.

## Overview of Sandia National Laboratories ablation activities

Justin Smith<sup>a,\*</sup>

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## PRELIMINARY POST-TEST ABLATION ANALYSIS OF THE EXOMARS2016 SCHIAPARELLI MODULE DURING THE ENTRY ON MARS ATMOSPHERE

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**Introduction:** The EXOMARS 2016 mission was the first (of two) joint European-Russian mission aiming at searching the evidence of past extra-terrestrial life on Mars. After a successful launch of the Russian Proton rocket on the 14th of March, 2016, from Baikonur, and several liberation maneuvers while orbiting the Earth, the Breeze M upper stage carrying the Trace Gas Orbiter (TGO) and the Schiaparelli Entry Descent and Landing module started a long journey to Mars. Seven months later, on the 16th of October 2016, the space probe was released on a direct entry path to the red Planet. After a nominal entry and an expected aerodynamic braking, saturation of the GNC algorithm during the highly dynamic deployment phase of the parachute, led to a final free fall of the module and a destructive impact on ground.

However, telemetry of the entry phase was recorded and enabled a post-flight analysis of the heat shield behavior. This paper provides an initial assessment of the thermal instrumentation data that is comprised of in-depth temperatures in the TPS made of Norcoat Liege (a phenolic impregnated cork based ablator). In addition to an ablation scheme sensitivity analysis and material thermal diffusivity correction, a preliminary inverse analysis is performed where the time-dependent surface heating is estimated from flight-measured subsurface temperature data.

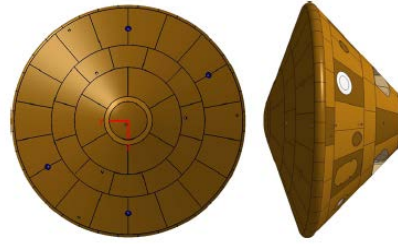
### Instrumentation and Aerothermodynamic database rebuilding:

The capsule aeroshell was a 2.4 m diameter spherically-blunted 70-degree half-angle cone with a truncated conic after body (Fig. 1). Schiaparelli's front and back heatshield was made of an ablative material called Norcoat Liege®. This material is made of cork granules impregnated with phenolic.

The thermal instrumentation consists in several thermopiles located in 3 different meridians separated by 120 deg.

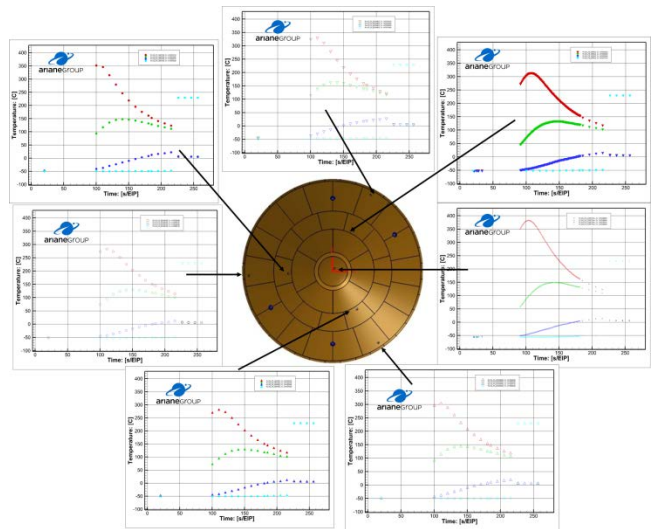
Thermal plugs are strategically placed from the stagnation region up to the shoulder to cover as much as possible all the possible effects of the angle of attack, lam-

inar to turbulent transition and wind relative velocity azimuth on the in-depth thermal response.



**Figure 1:** Front and side view of the 70 degree Schiaparelli entry probe.

Figure 2 presents an overview of the raw in depth thermocouples measurements as received from in board telemetry acquisition system.



**Figure 2:** In depth raw thermocouples readings on Schiaparelli front heat shield

After tuning the thermal and pyrolysis material model with direct thermocouple driving approach, an inverse algorithm involving a 1D finite element model of the plugs is run to retrieve the apparent net surface aero-



thermodynamic heat flux both on the front and back shield.

The preflight predictions of the aerothermodynamic loads based on engineering tools and the best estimate are then came up against the inverse total heat flux to increase model accuracy and refine the margin policy.

This data are compared with the imbedded DLR's environment instrumentation ( COMARS+) in order to validate the accuracy of the inverse approach.

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## Measurements of Pyrolysis Gas Interactions with Dilute Plasmas

P. Jagun, R. Herrmann-Stanzel, N. Martin, J. M. Meyers and D. G. Fletcher  
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**Abstract:** Extensive measurements of pyrolysis gas production from PICA and its substrate, Fiberform, have been conducted in the 30 kW Inductively Coupled Plasma (ICP) Torch Facility at the University of Vermont (UVM). Initial efforts focused on developing an injection probe that would allow the steady-state injection of pyrolysis gases through a porous carbon plug to simulate emission [1]. Plasma conditions for these tests consisted separately of pure argon and oxygen, nitrogen, air, and carbon dioxide diluted with argon. Argon dilution was critical for slowing down oxidation reactions and maintaining the ablative material surface location [2]. The first tests used emission spectroscopic measurements to characterize the pyrolysis interactions with the different reactive plasma gases for samples of PICA and Fiberform [2]. Subsequent tests were performed by injecting using different mixtures of H<sub>2</sub> and CO<sub>2</sub> through the porous graphite plug into the plasma stream and recording the spectrally resolved emission to compare with the PICA results. One such example comparison is shown in Fig. 1 for a dilute air plasma. The spectra overlap well for the molecular features: CN, OH, NH, but less favorably for the atomic features: H, Na. Note that sodium emission is strongly evident for all PICA sample tests.

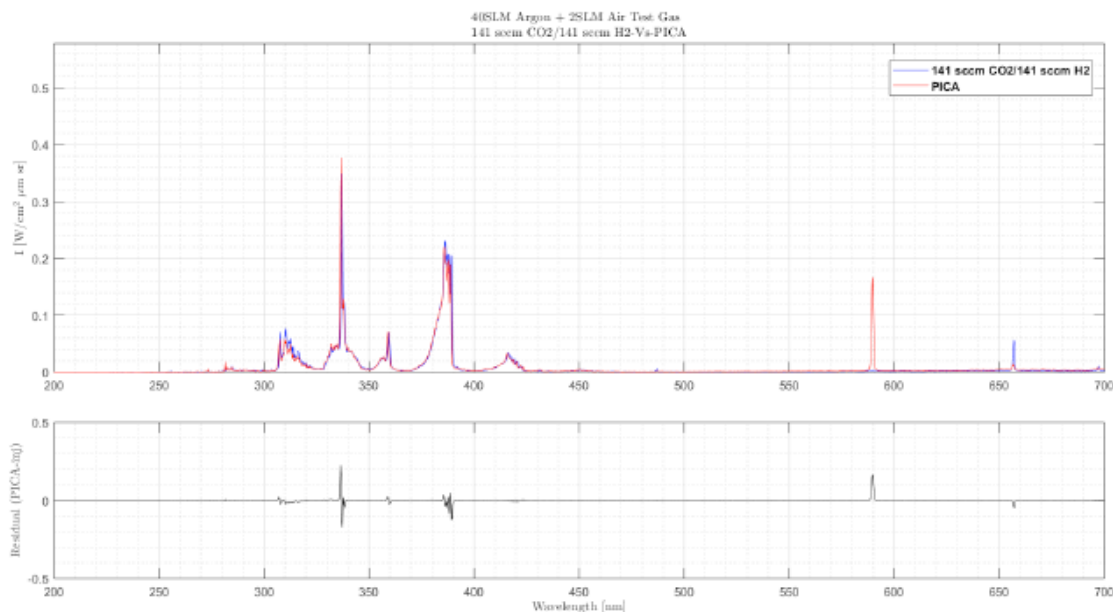


Fig. 1. Comparison of spectrally resolved emission from PICA pyrolysis with steady state injection of H<sub>2</sub> and CO<sub>2</sub> for a dilute air plasma test.

Results from similar tests will be presented at the workshop for other plasmas and for injection gas mixtures that replicate the emission measured from PICA. Additional

results from preliminary measurements of CO [3] and H using laser-induced fluorescence (LIF) will also be presented. These measurements represent spatially resolved measurements of the pyrolysis gas reactive species. These measurements are being used to validate chemical kinetics models used in current CFD codes [4].

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## **DETERMINATION OF THE ABLATION PROPERTIES OF A NEW CLASS OF ABLATIVES BY MESA CODE**

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### **ABSTRACT**

Ablative materials that are exposed to various hostile environments such as solid rocket motors, missile launching systems, or thermal protection systems (TPS). These materials have been investigated and developed widely in the defense and aerospace industries. Performance of the systems depends on the determination and investigation of ablative properties of new materials. In this study, MESA (Material Erosion and Stress Analysis Code) developed at Pennsylvania State University by F.B. Cheung and B.C. Yang is used for the determination of the ablation properties of a class of glass/phenolic composites. MESA code can predict mechanical erosion due to particle impact, thermochemical ablation due to imposed heat flux, thermal buckling due to internal pore pressure, and thermal studies in the ablative material. In addition to ablation properties, transient distributions of the local temperature, density and internal pore pressure can be obtained. Moving boundary due to surface recession is achieved by a time-dependent variable grid structure and suitable stretching factors. Variation of local temperature, internal pore pressure, density and mass flux related with flow of the decomposition gases inside the material are described by an axisymmetric cylindrical coordinate system. Numerical computation was conducted using the MESA code to predict the performance of ablatives, such as H41N and MXBE-350 and compared with the experimental data performed at FMC Corporation Naval Systems Division by F.B. Cheung and B.C. Yang [1, 2]. As a result, the MESA code was validated by comparing the numerical results with experimental results.

In this study, a two-dimensional material erosion and stress analysis (MESA) code is used for predicting the performance of high-temperature ablative materials. In the scope of this study, material response (MR) of MXB-360, a continuous strand randomly oriented fiberglass mat, impregnated with a filled phenolic resin, was used. Detailed thermophysical properties of MXB-360, such as mass loss, rate of mass loss, specific heat, heat of decomposition, thermal conductivity of virgin and char materials, thermal expansion, permeability, and porosity as a function of elevated temperature (up to 1,000°C) are provided by J. B. Henderson [3]. Surface temperature, in-depth thermal properties, and average recession results from the MESA code will be compared with the experimental data provided by J. Mendez *et al.* [4]. Mendez *et al.* conducted a set of experiments using The University of Texas at Austin's oxy-acetylene test bed with advanced diagnostics at a prescribed heat flux of 1,600 W/cm<sup>2</sup> for 25 seconds for three materials, MXBE-

350, MXB-360, and graphite [4]. Mass loss rate was measured by measuring the mass before and after it was exposed to the flame. The same was done for erosion rate. Table 1 below shows the change in mass for each material, while Table 2 contains the data for erosion. These are average values of at least six identical tests.

Table 1. *Summary of Mass Loss Data*

Material	Initial Mass (SD) (g)	Final Mass (SD) (g)	Total Mass Loss (SD) (g)	Total Mass Loss (SD) (%)	Mass Loss Rate (SD) (%/s)
MXBE-350	3.77 ± 0.13	2.55 ± 0.09	1.22 ± 0.08	32.3 ± 1.5	1.29 ± 0.06
MXB-360	4.27 ± 0.08	3.19 ± 0.06	1.08 ± 0.08	25.3 ± 1.6	1.01 ± 0.06
Graphite	3.75 ± 0.07	3.60 ± 0.08	0.15 ± 0.02	4.0 ± 0.7	0.16 ± 0.03

Table 2. *Summary of Erosion Data*

Material	Initial Thickness (SD) (mm)	Final Thickness (SD) (mm)	Total Erosion (SD) (mm)	Total Erosion (SD) (%)	Erosion Rate (SD) (%/s)
MXBE-350	9.78 ± 0.02	6.60 ± 0.81	3.18 ± 0.81	32.5 ± 8.3	1.30 ± 0.33
MXB-360	10.23 ± 0.02	7.30 ± 0.83	2.93 ± 0.83	28.6 ± 8.1	1.14 ± 0.32
Graphite	10.04 ± 0.10	9.89 ± 0.14	0.15 ± 0.06	1.5 ± 0.7	0.06 ± 0.03

As seen in the Table 1, both composite materials experienced a significant mass loss when exposed to the flame. Overall, MXBE-350 experienced the greatest mass loss, followed by MXB-360. Almost no mass loss was seen with the graphite samples, who on average loss ten times less the amount of mass than the other materials. The erosion rate, shown in Table 2, followed a similar pattern. MXBE-350 experienced a slightly greatest erosion rate than MXB-360. Graphite once again saw little change. These data will be used to validate our “material response” model of MXB-360 composite.

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## Thermogravimetric analysis of phenolic and silicone decomposition products

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### Abstract

Spacecraft entering planetary atmospheres require sophisticated low-density thermal protection systems (TPS) that reduce heat flux to efficiently protect the vehicle payload. Low-density carbon/phenolic materials are typically chosen for extreme applications because they are lightweight and have outstanding insulation capabilities. Most common within this class are the rigid, low-density phenolic-impregnated carbon ablators (PICA) used on the Stardust and Mars Science Laboratory (MSL) aeroshells. A commercialized version, PICA-X, was flown by Space-X on the Dragon capsule. Recently, silicone-based materials have been coupled with carbon/phenolic composites for TPS applications. Notable examples in the MSL were RTV-560, used as gap filler between PICA tiles, and NuSil CV-1144-0 applied as a sprayed-on coating to seal PICA and suppress dust during clean-room operations.

To make best use of the MEDLI (MSL Entry, Descent & Landing Instrument) flight data for validating material response models, it is important to account for the effects of RTV-560 and NuSil decomposition with PICA ablation. There are no high-fidelity models for the decomposition of those materials, and experimental data is scarce. Our goal is to provide experimental data to support MEDLI data analysis and prepare for MEDLI2, which is part of the Mars 2020 instrumentation suite. We report on the status of a new effort aimed at collecting modern data on both silicones and phenolics to feed state-of-the-art ablation codes.

We used a Netzsch thermogravimetric analysis (TGA) apparatus equipped with a residual gas analyzer (RGA) mass spectrometer (MS) system to explore the pyrolysis gases generated during high-temperature decomposition of phenolics and silicones up to 1600 K. The system is interfaced to the MS system via a 3-m long, 100- $\mu$ m internal diameter (ID) heated capillary, which introduces the pyrolysis products into our dual mass spectrometer system. This contains both a time-of-flight mass (TOF) spectrometer for single-photon ionization (SPI) and an RGA for typical electron impact (EI) measurements—a combination that is very useful for analyzing pyrolysis products.

We will describe our TGA-MS measurements for mixtures of phenolic resins and silicones and the development of a quantification method based on a ‘ladder’ quantification procedure to evaluate the resultant gas-phase mole fractions of decomposition products. We will present our initial results, discuss the challenges of quantification, and compare to preliminary models.

**Keywords:** Pyrolysis, Phenolics, Silicones

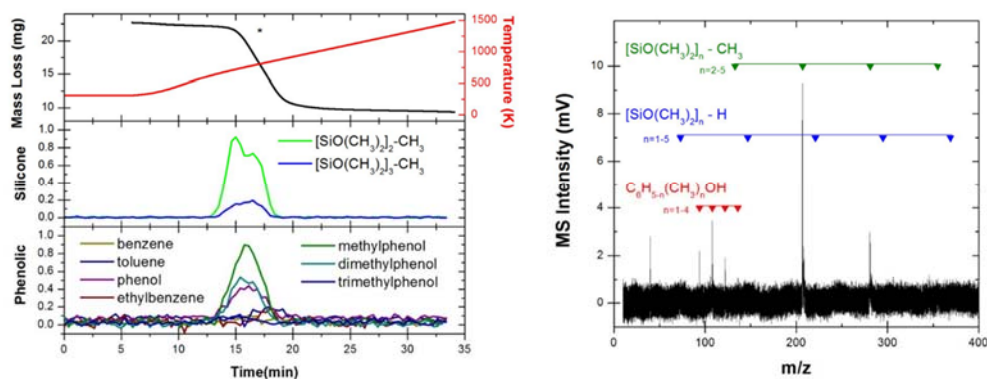


Figure 1. The TGA mass loss and corresponding SPI data for key silicone (middle-left panel) and phenolic (middle-bottom) products. Right panel shows the SPI-MS data over time as represented by the asterisk above the TGA curve. Peaks are identified by siloxane species missing a methyl group (green), missing a hydrogen (blue), and by phenolic products (red).

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# Molecular Beam Studies of Carbon and Silicon Carbide Ablation by Atomic Oxygen

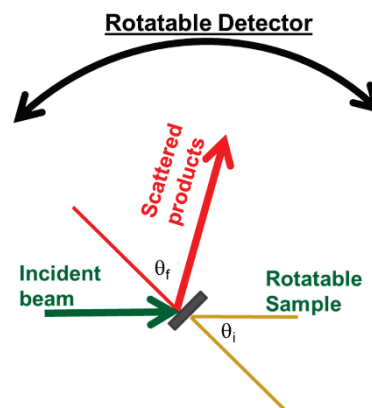
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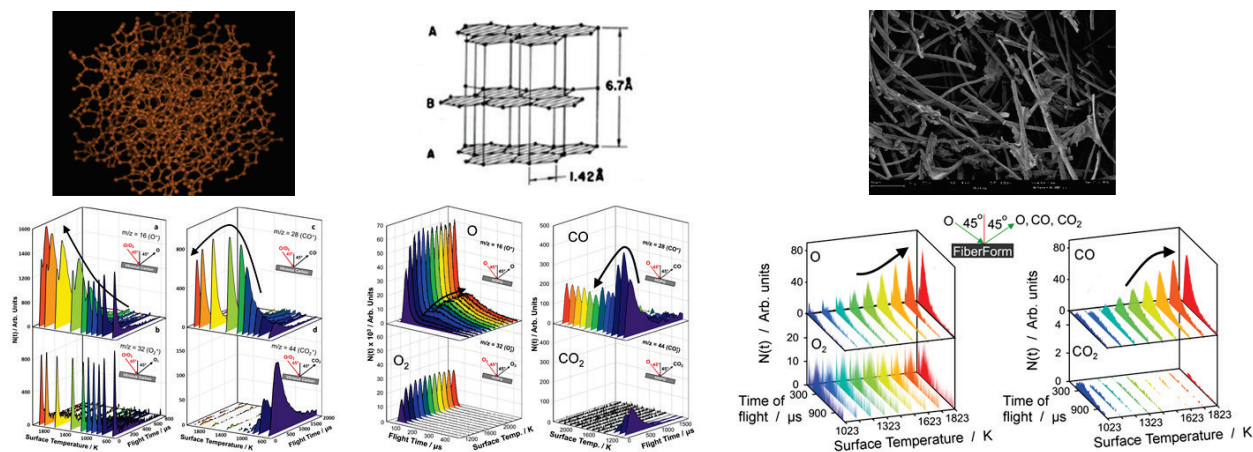
## Abstract

Understanding the oxidation mechanisms of heat shields is key to reliable design with low uncertainties. We have been using molecular beam-surface scattering experiments (see Fig. 1) to gain an understanding of the high temperature oxidation of model materials.[1-4] We have conducted extensive investigations of three types of carbon, (1) highly oriented pyrolytic graphite (HOPG), (2) vitreous carbon, and (3) carbon fiber preform (FiberForm), and new work is underway to understand the detailed oxidation mechanisms of silicon carbide (SiC).

The experiments are performed with a laser-detonation molecular beam source that produces ground-state O and O<sub>2</sub> with a mole ratio of approximately 90:10 and a nominal velocity of 8 km s<sup>-1</sup>. The vitreous carbon and FiberForm samples are heated resistively, and the HOPG and SiC samples are heated radiatively by placing the sample in close proximity to a resistively heated vitreous carbon sample. The products that scatter either reactively or non-reactively from the surface are recorded with a rotatable mass spectrometer detector operating in a pulse counting mode. The primary data are number density distributions as a function of arrival time at the detector, with a particular incident angle ( $\theta_i$ ) and final angle ( $\theta_f$ ). These number density distributions are referred to as time-of-flight (TOF) distributions. These distributions allow the simultaneous characterization of the products and the timescale of the reactions. The data are able to distinguish between products that scatter on a timescale too short for thermal equilibrium to be attained (impulsive scattering in the case of non-reactive scattering, and Eley-Rideal in the case of a reaction) and products that desorb in thermal equilibrium with the surface (trapping desorption in the case of non-reactive scattering, and Langmuir-Hinshelwood in the case of reaction).



**Figure 1.** Schematic diagram of beam-surface scattering experiment.



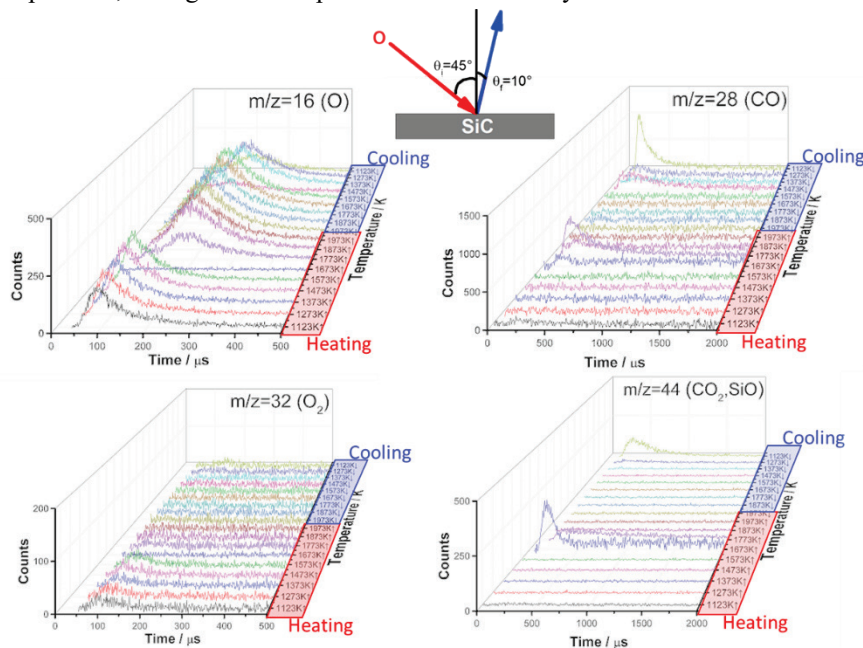
**Figure 2.** Time-of-flight distributions of O, O<sub>2</sub>, CO, and CO<sub>2</sub> products scattering from three types of carbon as a function of surface temperature. The O<sub>2</sub> is not from O-atom recombination, but rather from direct scattering of O<sub>2</sub> that is in the incident beam.

The reactive scattering dynamics on all three carbon surfaces are similar yet the details of the dynamics differ (Fig. 2), suggesting that the oxidation mechanisms on all sp<sup>2</sup> types of carbon are similar but that surface morphology influences the relative importance of the individual mechanisms. Furthermore, the data indicate that the reaction mechanisms occur in thermal equilibrium with the surface and that the surface oxygen coverage is high except at the



highest temperatures; therefore, the beam-surface scattering data are relevant to hypersonic gas-surface interactions. In general, we have learned that incoming O atoms increase surface coverage and lower the barriers to CO and CO<sub>2</sub> formation. Increasing surface temperature promotes reactions as long as sufficient O is present. At high temperatures, desorption of O and CO lowers the surface coverage of O, which increases reaction barriers and reduces the number of surface O atoms that are available for reaction, thus lowering the reactivity of carbon with O atoms. A higher flux of O atoms on the surface can maintain the surface coverage of oxygen and allow high reactivity even at higher temperatures. There are both prompt and slow processes that lead to the production of CO reaction products, and the rates of all these processes must be considered in a finite rate model for CFD.

In the new experiments on SiC, we have used 6H single crystal surfaces and have started by oxidizing these surfaces in the atomic oxygen beam to produce an SiO<sub>2</sub> layer that is approximately 5 nm thick. Upon heating in vacuum, the oxide layer decomposes quickly at a temperature of ~1400 °C and produces volatile SiO. As the sample is heated further, no more SiO is produced and a graphitic carbon layer remains with a thickness indicative of more than 10 layers of graphene (determined by Raman analysis of a sample that has been heated and then cooled to room temperature). When the atomic oxygen beam is directed at the oxidized SiC surface (see Fig. 3), no reaction products are observed until the surface temperature increases above 1400 °C where the oxide layer is removed. This is thus the transition temperature from passive to active oxidation. Above this transition temperature, the scattering dynamics are indicative of scattering from graphitic carbon (similar to what we observed on HOPG). Apparently, the O-atom flux of our beam is not sufficient to remove the graphitic layer on the time scale of our experiments. Further experiments are underway to investigate the detailed reaction mechanisms in the active oxidation regime with a higher O-atom flux. In addition, additional experiments are planned to study the reaction mechanisms that occur at the transition temperature, during the decomposition of the oxide layer.



**Figure 3.** Time-of-flight distributions of O, O<sub>2</sub>, CO, and CO<sub>2</sub>, SiO products scattering from oxidized SiC as a function of surface temperature. The O<sub>2</sub> is not from O-atom recombination, but rather from direct scattering of O<sub>2</sub> that is in the incident beam.

Keywords: Molecular beam, atomic oxygen, carbon oxidation, silicon carbide oxidation

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# Predictive Modeling of Chemical and Structural Failure of Porous Ablative Materials

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## Abstract

Recent post-flight analyses of atmospheric entry vehicles, such as the Mars Science Laboratory (MSL) [1,2], have revealed that current ablation models are highly conservative, therefore motivating further development. During the past decade, significant advances in predictive ablation modeling have been made. For example, models are now capable of resolving the thermal protection system (TPS) microstructure, as well as predicting the flow physics and gas-surface chemistry within porous microstructure. However, predictive modeling approaches for the structural response of the TPS are currently missing. Modeling TPS structural response is a considerable challenge, since the structural response and possible failure of the TPS is tightly coupled to both the chemical processes (such as oxidation) occurring on the microstructure and the boundary layer aerothermodynamics (shear stress and heat flux). The goal of the proposed research is to develop a predictive modeling capability that couples thermochemical TPS response with its microscale thermo-structural response. Such a capability would enable precise assessment of TPS microstructure response, including complex processes such as spallation, and could ultimately be used in the design of new TPS materials at the microstructure level, such as new woven TPS currently under development at NASA [3,4].

The research is a collaborative project between the University of Minnesota and the University of Kentucky, including interaction with NASA. At Minnesota, research focuses on molecular simulations of boundary layer flow over resolved microstructure using the direct simulation Monte Carlo (DSMC) method. Boundary layer profiles are extracted from CFD solutions from relevant flight conditions and these flow profiles are used to initialize targeted DSMC simulations of flow over resolved microstructure. This is depicted in Fig. 1 where a CFD solution corresponding to the Stardust re-entry vehicle is extracted and used to initialize a DSMC simulation of flow over a fiber-based TPS geometry. The DSMC simulation is able to resolve traction forces and heat flux locally on the microstructure surface, in addition to the flux of reactive species (such as O atoms). These fiber-level properties are then analyzed by the University of Kentucky team using thermo-structural response calculations of individual fibers. Stress fields are computed and analyzed to identify locations and magnitudes of peak values. In addition, research at the University of Kentucky will use the local flux of reactive species to the surface, as calculated by DSMC, and develop an oxidation model that includes the complex process of pitting. The combination of microstructure weakening due to oxidation with thermo-structural effects will ultimately be used to predict various failure mechanisms of the TPS. The overall predictive capability could be useful for understanding spallation, and failure mechanisms of a variety of carbon-based TPS.

**Keywords:** Hypersonics, Ablation, Microstructure.

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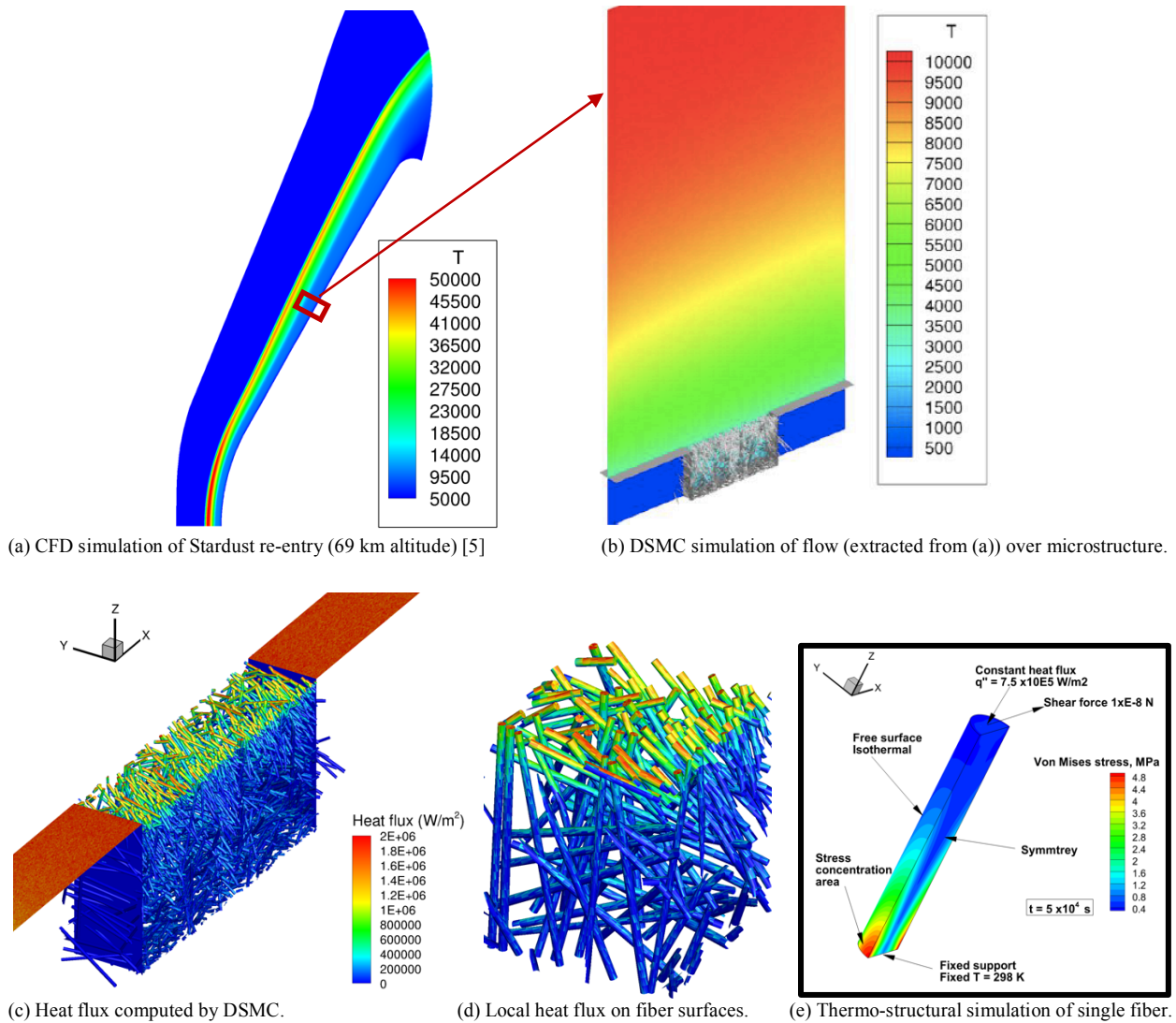


Figure 1: Multiscale approach to predicting thermos-structural response of carbon microstructure under relevant hypersonic conditions.

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## Pitting dynamics in carbon oxidation

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### Abstract

In order to understand pitting (formation of cavities) in carbon oxidation, we have used accelerated Monte Carlo simulations together with a simple kinetic mechanism, which nevertheless incorporates the essential surface processes controlling oxidation. We have studied the evolution of the surface topology and more specifically the growth rate of cavities (pits) and we show how these depend on the energetics of the surface processes.

**Keywords:** Carbon oxidation, ablation, pitting

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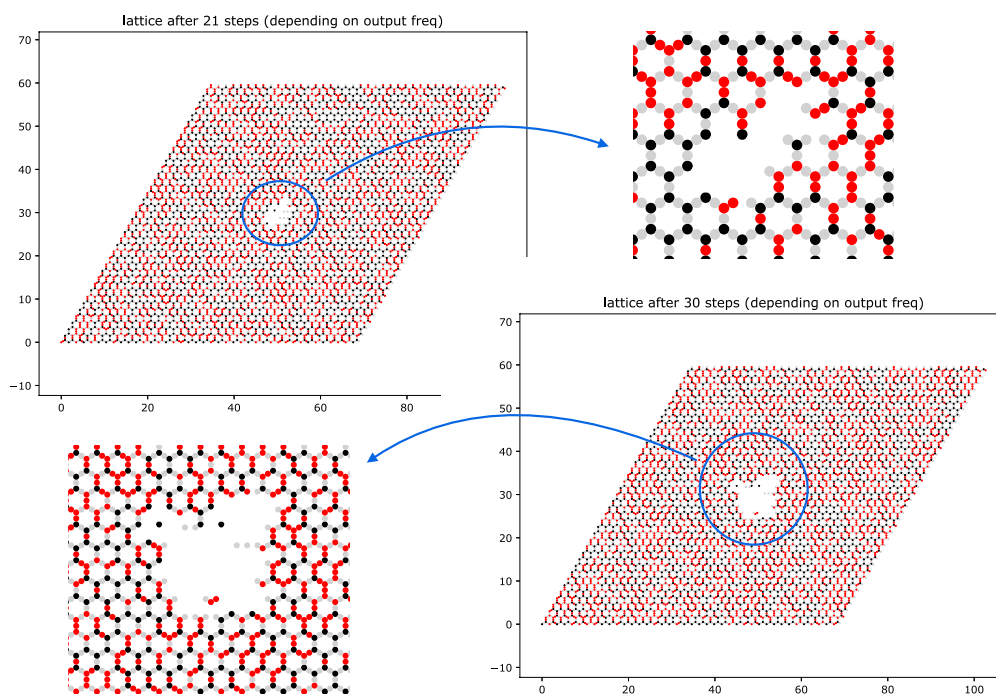


Figure 1: Snapshots of the structure a pit on graphene during oxidation.

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# Apparent permeability prediction on micro-porous media with the lattice Boltzmann method

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## Abstract

Thermal protection systems (TPS) play a crucial role in the atmosphere re-entry stage of a spacecraft concerning thermal energy dissipation. Their micro-porous structure enable hot atmosphere gases to flow through and initiate pyrolysis and ablation to scatter friction generated heat [1]. However, they take a significant part in the total launch weight [2] : optimizing them has thus become a critical issue in reducing spacecraft launch costs. To assess their efficiency, one must preliminary look at the gas flow behaviour, which can be measured by computing its permeability through TPS.

Adapted models must be used, because the combined effects of low pressure gases at high altitude (also known as *rarefied gases*) with micro-porous flows make the usual continuous flow assumption invalid. Furthermore, properly capturing rarefied effects such as slippage at solid walls is fundamental for accurate permeability prediction, as its value in rarefied flow regimes significantly derives from the continuous one. Rarefaction is characterized by the Knudsen number  $Kn = \frac{\lambda}{H}$ , with  $\lambda$  the mean free path of the gas, and  $H$  the characteristic length of the flow region, and flow regimes can be classified according to  $Kn$  [3].

Within this framework, we consider the lattice Boltzmann method (LBM) as a mechanism to tackle small-scale flows through TPS, since promising results have been shown in rarefied gas simulations [3] and through complex porous media [4]. Permeability is calculated here with LBM through structured 2D granular media in rarefied regimes. Initial results show that LBM is able to capture the rarefaction influence on permeability, as the numerical results are in good agreement with Klinkenberg primary observations [5].

**Keywords:** Permeability, Porous media, Rarefied Gases, Lattice Boltzmann, Klinkenberg effect

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## 1. Methodology

### 1.1. Rarefaction influence on permeability

As the flow becomes rarefied, slippage effects occur at solid walls, resulting in an increased flow rate. Based on Darcy's law for creeping flows, the computed permeability also increases, and is referred to as the Klinkenberg effect. Several correlations have been developed, based on theoretical [6, 7] and numerical work [8, 9]. The apparent permeability  $K_a$  for rarefied flows can be generally expressed as  $K_a = K_\infty f_c(Kn)$  where  $f_c(Kn)$  is the correction factor due to rarefaction and  $K_\infty$  is the intrinsic permeability predicted by Darcy's law in the continuous regime.

### 1.2. Rarefied boundary conditions

The bounce-back boundary condition commonly used in the standard LBM algorithm fails to simulate slip velocity at solid walls. To take rarefaction effects into account, a diffuse bounce-back boundary condition (DBB), combination of bounce-back and diffuse reflection boundary conditions, is thus implemented. Based on the kinetic theory, the diffuse reflection boundary condition lies on the idea that a proportion (identified by a coefficient *beta*) of the impinging distribution functions  $f_i$  capture the wall's density and velocity, before being scattered back following a Maxwellian distribution :  $f_i(t_{n+1}) = (1 - \beta)f_i^{BB}(t_n) + \beta f_i^{DBB}(t_n), \beta \in [0, 1]$ .

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### 1.3. Effective viscosity

Intermolecular collisions become less frequent because of gas rarefaction, increasing  $\lambda$  (and thus  $K_n$ ). Solid boundaries must also be taken into account when rarefaction rate increases, as the fluid molecules near them have smaller  $\lambda$ . It can be achieved by implementing a "wall function"  $\psi$  (set to  $\psi(K_n) = \frac{1}{1+2K_n}$  here based on [3]), which weights the unbounded mean free path. Numerically speaking, it leads to a change of the relaxation coefficients  $\tau_i$  in the collision operator in LBM which are related to the dynamic viscosity  $\nu$ . The  $\nu$ - $K_n$  relationship becomes then  $\nu = \sqrt{\frac{2}{3\pi}} K_n H \psi(K_n)$ .

## 2. Preliminary results

The changes in LBM for rarefaction effects implemented, simulations are now performed on 2D structured arrays of square and circular cylinders with staggered and inline arrangements as pictured in figure 2 in [4] for different porosity  $\phi$  and  $K_n$  values. The computed  $f_c$  are plotted against the existing correlations at figure 1 and show that LBM can predict  $K_n$  influence on  $K_a$ , since the numerical results lie within the range of values predicted by the references.

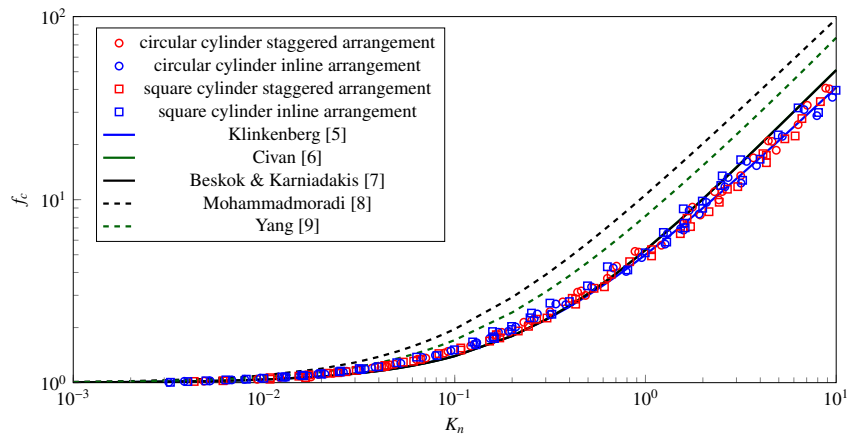


Figure 1: Correction factor for apparent permeability against  $K_n$

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# Modeling the Effective Thermal Conductivity of Anisotropic Porous Materials

Abstracts of the 10<sup>th</sup> Ablation Workshop, University of Vermont, September 17-18, 2018

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## Abstract

Effective design of ablative thermal protection systems, used to protect spacecraft during the severe aerothermal conditions of atmospheric entry, requires high-fidelity material response models. Due to the highly porous nature of light-weight materials used in NASA's spacecraft heatshields, micro-scale modeling has become an important component of this effort. One of the main focuses in micro-scale modeling of heatshield materials is predicting the effective thermal conductivity of the bulk material, often difficult to determine experimentally. This is a critical parameter needed in macro-scale material response computations of thermal protection systems. The state-of-the-art in micro-scale modeling consists of performing thermal transport simulations based on computational grids that resolve the micro-structure of the material, as in grids obtained from high-resolution computed tomography. Numerical schemes are under active development at NASA for computing the effective thermal conductivity of porous materials, based on 3D tomography images of the material and the conductivity of its constituting phases. A common assumption is that the thermal conductivity of these phases is isotropic. Although this assumption is valid for the pore-filling gas, it may not be accurate for carbon fibers, such as those used in carbon/phenolic ablators, especially if they come in a directional weaving pattern. This project focuses on the development of a fully-conservative finite volume scheme based on a refinement of the prominent Multipoint flux approximation (MPFA) technique [1]. This is used to compute the effective thermal conductivity of a material accounting for the anisotropy of its constituents. This capability is implemented in the Porous Microstructure Analysis software, PuMA [2]. The effort utilizes X-ray micro-tomography to provide high resolution representations of the material, upon which simulations are conducted. The 2D implementation was verified against several analytical steady-state solutions, one of which is shown in Figure 1.

## Keywords:

Steady-state Heat Conduction, Anisotropic Discontinuous Diffusion Tensors, Porous Media, Micro-tomography, PuMA, Cartesian Grid, Finite Volume, Effective Thermal Conductivity

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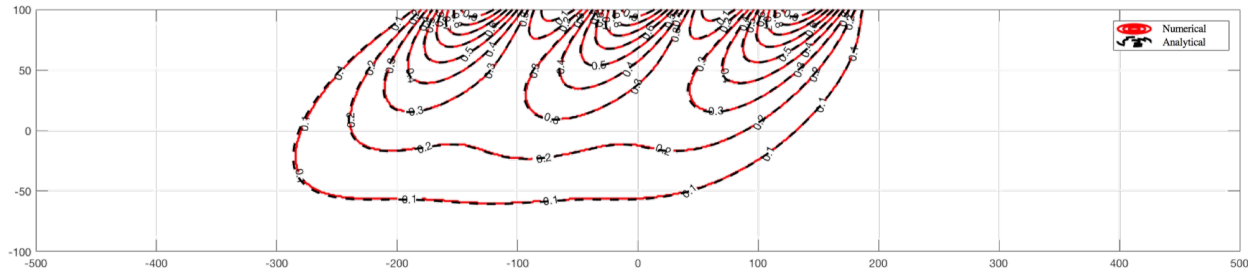


Figure 1: Comparison between analytical [3] and numerical solutions of a cosine temperature profile applied on the surface of an anisotropic strip.

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## KATS-Universal Solver: Application to flow tube oxidation modeling

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### Abstract

The CFD/Material response KATS-US is used to model a series of flow tube oxidation experiments. For each experiment, a FiberForm<sup>®</sup> sample is inserted in the middle of a flow tube, maintained at a constant temperature and at a constant mass flow rate for about 10 minutes. The upstream and downstream pressures are recorded. The recession and the final mass of the sample are measured after each experiment. With the provided data, the oxidation is modeled using KATS-US framework by solving free flow and solid material in the same computational domain. Several assumptions were made to simplify the equations and to speed up the simulation, but KATS-US successfully predicted the recession and the gas species diffusion in a tightly coupled manner, as shown in the figures. At  $T \approx 1500\text{K}$ , the  $\text{O}_2$  oxidation is mainly a surface phenomenon, while the  $\text{CO}_2$  oxidation occurs at in-depth of the material, and part of the  $\text{CO}_2$  diffuses through the test sample. These simulations are consistent with the observations from the modeled experiments.

**Keywords:** FiberForm<sup>®</sup>, Oxidation, Validation

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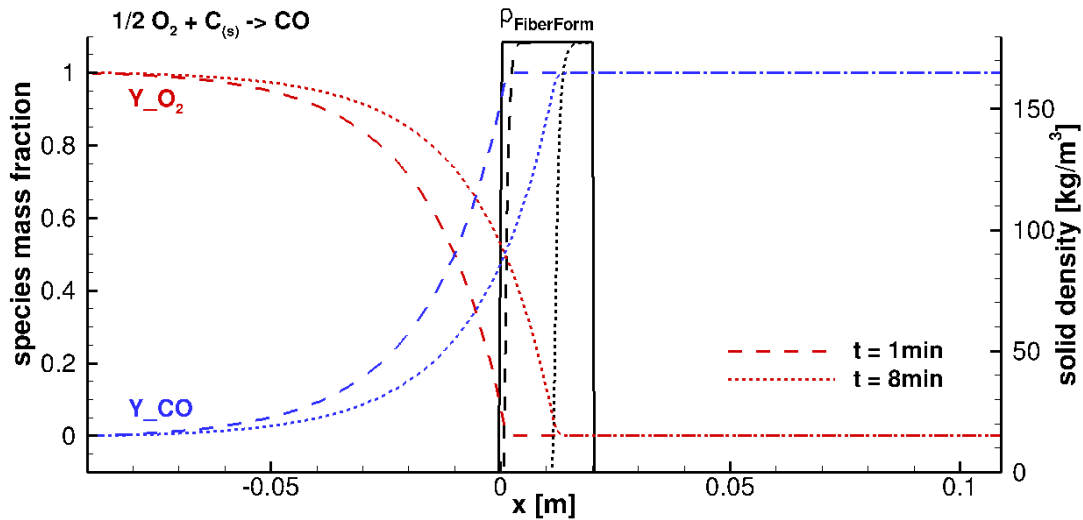


Figure 1: KATS-US results of  $\text{O}_2$  oxidation at  $T=1502\text{K}$

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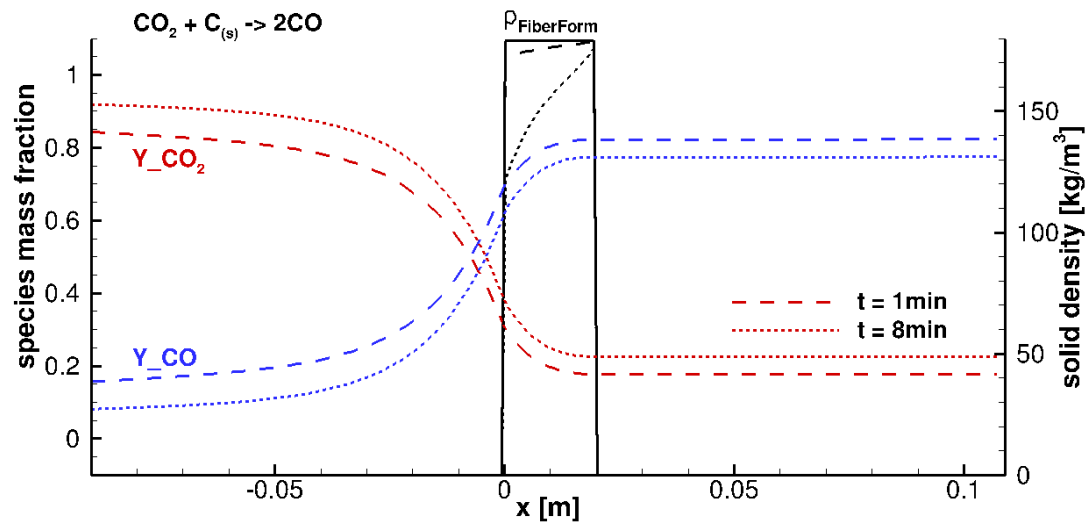


Figure 2: KATS-US results of  $\text{CO}_2$  oxidation at  $T=1508\text{K}$



## Effect of Carbon-based Ablation Products on Hypersonic Boundary Layer Stability

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### Abstract

From Prandtl to present day, fluid dynamicists have been working to understand and predict the behavior of the viscous boundary layer, especially transition from laminar to turbulent which has a significant impact on aspects of vehicle design such as the Thermal Protection System. As understanding and theories of boundary layer stability developed, morphing from incompressible to compressible and adding higher mode disturbances, the complexity and interdependence of stability of the boundary layer on the physics of the flowfield properties and vehicle characteristics have become evident. At hypersonic velocities, the stability of the boundary layer becomes mainly dependent on pressure gradient, crossflow disturbances and ablation, which includes the blowing rate as well as how ablation changes the chemical composition of the boundary layer[1]. With high heat transfer rates and smooth ablation characteristics, many hypersonic vehicles use carbon surface ablators, which introduce  $C$ ,  $C_2$ ,  $C_3$ ,  $CO$ ,  $CN$  and  $CO_2$  into the flow. The presence of  $CO_2$  has a damping effect on second mode instabilities, the primary instability in supersonic boundary layers [2, 3].

A Computational Fluid Dynamics (CFD) study was accomplished using gas-surface reaction models developed by Park [4, 5, 6], Zhukov and Abe (ZA) [7], and a modification to the ZA model[8]. The variation of the modified ZA (MZA) from the ZA model includes the use of mobile surface site calculations for the equilibrium constant and specified reaction rates for desorption of oxidation and nitridation [8]. The gas-surface models were used as a boundary condition using the US3D code, a finite-volume, chemically reacting Navier-Stokes CFD code developed by the University of Minnesota. The stability of the boundary layer was examined using a Linear Stability Theory (LST) code, STABL3D, developed by VirtusAero in collaboration with the University of Minnesota [9].

A simple 0.5 inch, 10 degree half-angle cone with a length of 50 inches was chosen for the study due to the simplicity of the geometry while still allowing for sufficient ablative surface area. The free-stream flow characteristics were based off standard atmospheric conditions at 30k feet and a velocity of 6 km/s, giving an edge Mach number of 9.

Figure 1(a) below shows the concentration of  $CO_2$  in the boundary layer using the different chemical models. The ZA model shows a significantly larger amount of  $CO_2$  in the boundary layer as compared to the other models. The Park models show only a very small concentration of  $CO_2$  in the boundary layer flow. The MZA model produces less  $CO_2$  than the ZA model due to the favoring the production of  $CO$  over  $CO_2$ .

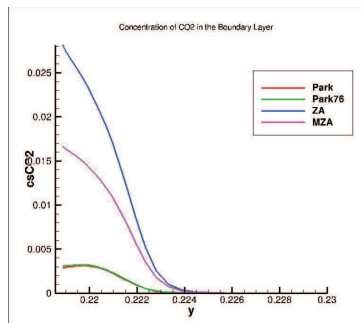
Figure 1(b) compares the maximum N factor, or amplification factor, for the different models. The ZA and MZA both show lower amplification rates than the Park models corresponding to the differences in the mass flux of  $CO_2$ . The ZA model produces significantly more  $CO_2$  in the flow than the other models. However, this increased concentration does not correspond to a linear relationship, and shows only a slight decrease in the amplification rate despite an order of magnitude larger concentration of  $CO_2$ . Similarly, the MZA model showed the least amount of amplification which does not correspond directly to the  $CO_2$  concentration.

Using the MZA model, it was possible to isolate the effect of the vibrational modes in the flow. The MZA model showed the least amount of amplification including chemical and vibrational terms. When the same flow was analyzed without the vibrational terms included, the results of the stability analysis shows a rise in the amplification factor. Without the vibrational modes to absorb the energy, the disturbances are allowed to grow larger, though at the same location along the body. Figure 1(c) shows a direct correlation between the vibrational energy absorption and maximum amplification. The link between vibration energy absorption and amplification rate is apparent.

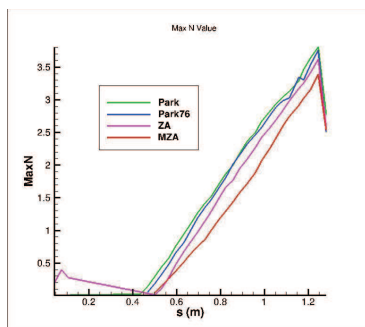
The impact of the chemical composition of the boundary layer as a result of surface ablation has an effect on the

stability of boundary layer. The ability for  $CO_2$  with its multiple vibrational modes excited at relatively low temperatures to absorb energy stabilizes the flow. Further simulations need to be conducted to determine the interdependence of other aspects, such as surface temperature, free-stream Mach, and blowing rates, need to be conducted to fully understand the effect of ablation products on boundary layer stability and how best to model this effect for transition prediction.

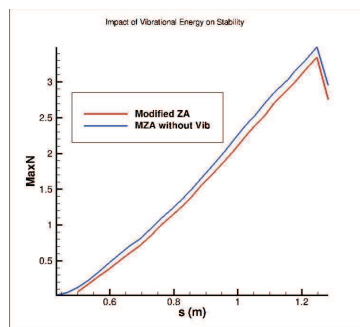
**Keywords:** Boundary Layer Stability, transition, ablation product, gas-surface chemical model, vibrational damping



(a) Concentration of  $CO_2$  in the Boundary Layer



(b) Maximum N Factor



(c) Vibrational Effects (Modified ZA Model)

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## Mesoscale Framework for Multi-Physics Simulation of Ablative Thermal Protection Systems

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### Abstract

Ablative Thermal Protection Systems (TPS) are used to protect space vehicles during atmospheric entry. The ablation increases their ability to resist heat transport. The TPS of interest in this study is the Phenolic Impregnated Carbon Ablator (PICA) material, a composite made of a polymer resin matrix and carbon fibers. During the heat transfer, oxygen diffuses into the PICA structure and reacts with the carbon fiber as well as the resin. There are many chemical and physical reactions involved in the pyrolysis and ablation processes throughout the material volume. In this presentation, we present our preliminary efforts to develop a state-of-the-art mesoscale model of PICA ablation and pyrolysis. The mesoscale resolution of the PICA microstructure contributes to a better understanding of the rate of the pyrolysis and ablation processes. Moreover, it can be coupled with macroscopic simulations to provide more accurate results and reduce safety margins for operations. The phase-field model is being developed using the MOOSE Framework, an open-source Finite Element Method (FEM) solver. The preliminary study of oxygen reacting with a carbon fiber and generating chemical products demonstrates the feasibility of the mesoscale framework to model ablative TPS.

**Keywords:** Phase-field, Ablation, MOOSE Framework, Finite Element Method, Phenolic Impregnator Carbon Ablator, Thermal Protection Systems

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## Overview of the material response code MABLE

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### Abstract

The Multiscale ABLation Evaluation tool (MABLE) is a modular software package for modelling porous reactive materials. MABLE operates on three-dimensional unstructured grids and discretises the system state using the finite volume method. MABLE is under active development by Fluid Gravity Engineering (FGE) in the UK.

This presentation will provide an overview of the models currently implemented within MABLE. In particular, the presentation will discuss the model used to perform shape change and the use of the multi-point flux approximation (MPFA) to calculate face fluxes [1]; the latter is in the process of being implemented in MABLE.

**Keywords:** material response code, ablation, pyrolysis, porous media

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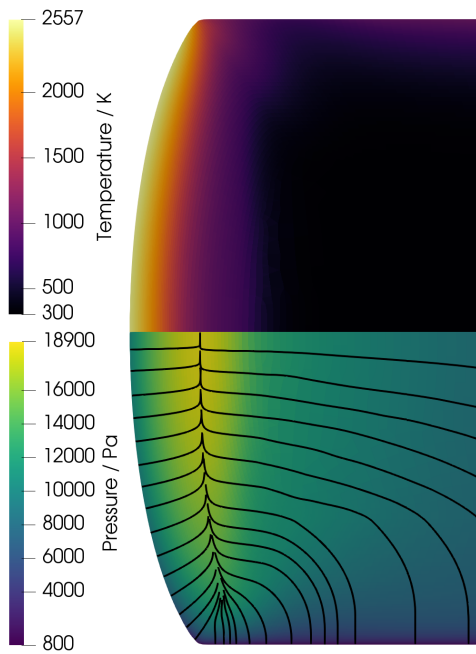


Figure 1: Demonstration arc jet run of a pyrolysing TACOT sample in an arcjet. Gaseous flow streamlines are shown in the bottom half of the figure.

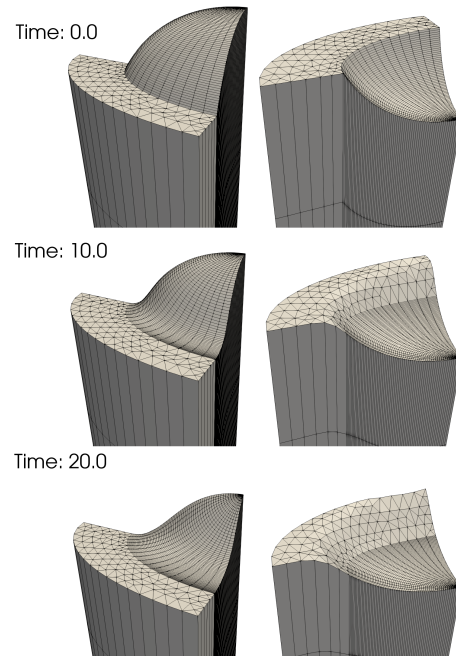


Figure 2: Demonstration of the shape change model acting on an elliptically shaped protrusion [left] and indentation [right] where the surfaces have constant recession rates.

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## Investigation of Factors Affecting Rocket Nozzle Conjugate Ablation Predictions

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### Abstract

Results from a series of fully-coupled, conjugate, two-dimensional simulations modeling the ablation of pyrolyzing carbon-phenolic material in the HIPPO nozzle [1] test case will be presented. These conjugate ablation studies investigate the effects of surface energy balance treatment, turbulence model, and radiation on the ablation predictions.

The conjugate analysis methodology utilized in this work couples the LeMANS flow solver [2, 3] to the multidimensional MOPAR-MD [4, 5] ablation and material response code in order to capture mutual interactions between the reacting flowfield and the ablating nozzle wall [6, 7]. The pressure trace for a rocket motor firing is divided into a number of discrete time points; the LeMANS flow solver is used to obtain a steady-state flowfield solution at each point. The wall boundary conditions required by the flow solver are obtained from MOPAR-MD, which performs a transient material response analysis starting from the solution obtained at the previous time point. At each time point the LeMANS flow solver and the MOPAR-MD material response solver work in an iterative fashion.

Multiple treatments of the surface energy balance at the ablating wall, with increasing levels of fidelity, are investigated. The Noncatalytic Wall – Enthalpy Conductance (NCEC) method uses a noncatalytic wall boundary condition for the flow solver. Enthalpy conductance (enthalpy based heat transfer coefficient) is computed within the flow solver and passed to the ablation solver, where it is used in conjunction with  $B'$  tables to compute the thermochemical ablation heat flux. The higher fidelity Integrated Equilibrium Surface Chemistry (IESC) treatment computes the surface energy balance directly from the diffusive fluxes at the ablating wall, without making transport coefficient assumptions or requiring  $B'$  tables. The final method, the Finite Rate Surface Chemistry (FRSC) treatment, computes surface recession by modeling finite-rate heterogeneous reactions between the char and four gas-phase species:  $H_2O$ ,  $CO_2$ ,  $OH$ , and  $O$ . The FRSC treatment should provide improved accuracy when the equilibrium surface chemistry assumption is not appropriate, such as when lower surface temperatures exist.

Predicted surface recession distributions for the HIPPO nozzle are compared in Figure 1 to experimental measurements. Surface recession is strongly affected by the choice of surface energy balance treatment. The low-fidelity NCEC method significantly over-predicts recession, while the higher-fidelity IESC treatment provides the best agreement with the experimental data. It can also be observed that the ablation response is not strongly affected by the choice of turbulence model, with simulations employing the Menter SST model predicting slightly less recession than simulations using the Menter BSL model. The influence of radiative heat transfer on surface recession predictions is highly dependent upon the choice of surface energy balance treatment. For the NCEC treatment, including radiative heat transfer leads to significantly higher recession predictions. In contrast, including radiation produces only small changes to the predicted surface recession values for the IESC method. This difference is attributed to the transport coefficient approximation utilized by the NCEC method.

The conjugate analysis methodology utilized in this work comprehensively incorporates fluid-thermal-chemical processes relevant to nozzles and other high temperature components, making it possible to rigorously capture the strong interactions and interdependencies that exist between the reacting flowfield and the ablating material. As a result, improved analysis accuracy has been demonstrated.

**Keywords:** Ablation, Rocket Nozzle, Conjugate Analysis, Carbon-Phenolic, Radiation, Turbulence Model

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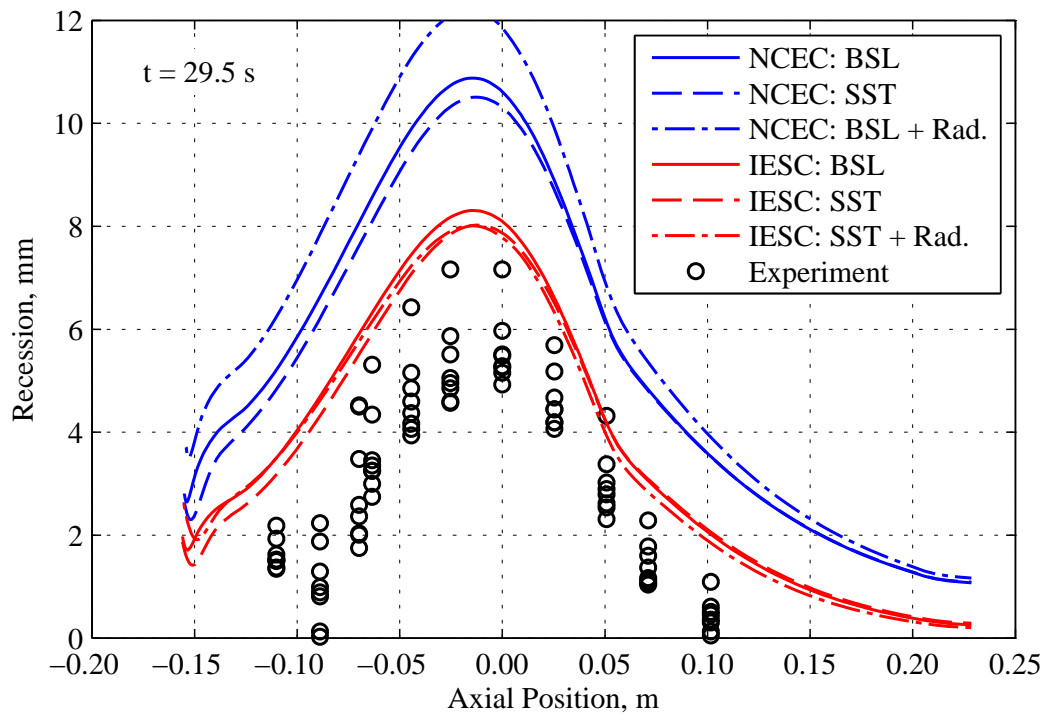


Figure 1: Comparison of predicted and measured final surface recession, demonstrating the effects of surface energy balance treatment, turbulence model, and radiative heat transfer on the predictions.

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## Icarus Material Response Modeling of Meteoritic Melt Interfaces: Application of an Atomistically-Derived Property Database

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### Abstract

During atmospheric entry, meteoroids are subjected to temperatures above the melting points of their constituent minerals, which leads to the formation of a molten surface layer. Ablation of the molten layer may occur either through vaporization or flow. The balance between these mechanisms relies heavily on the specific entry conditions [1] as well as the properties of the solid and molten meteoritic material. Here, we investigate the nature of meteoroid melt for three model systems (silica, enstatite, and chondrite) that have been examined through Arcjet experiments. [2] To do this, a melt flow boundary condition [1] is implemented in the Icarus material response solver to allow the examination of the thermodynamics of the solid/melt interface. Due to a lack of available property data at extreme conditions, *ab initio* techniques are used to develop a high-fidelity property database that includes thermal conductivity, viscosity, absorbance, reflectance, heat capacity, and melting point for the solid and liquid meteoroid models. [3] The so-determined properties are provided as an input database to Icarus, and the thermodynamics of the solid/melt interface at entry conditions are examined.

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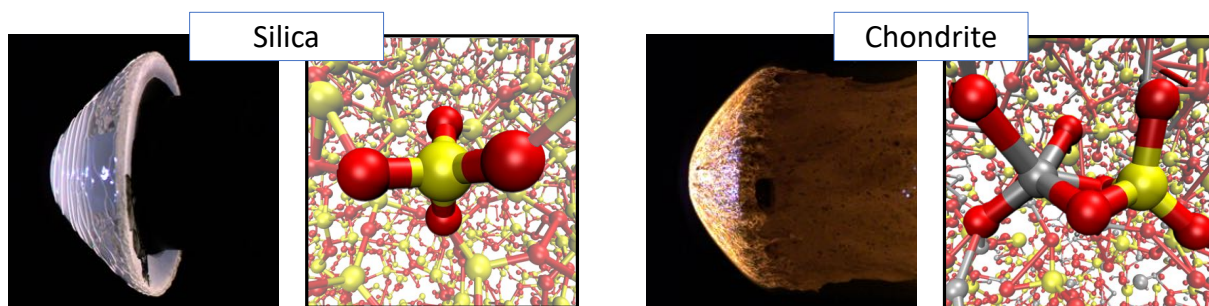


Figure 1: Arcjet and atomic simulation models of silica (*left*) and chondrite (*right*).

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## Mesoscale modeling of TPS materials: Effective property calculations and sensitivity analysis

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### Abstract

The performance of thermal protection systems (TPS) is dictated by mesostructural features of the composite governing its behavior in a complex multi-physical system coupling thermal transport, reactive fluid transport, and mechanical stress formation. Many commonly used engineering codes for ablation rely on volume-averaged material properties, which are only representative of a single material system and do not account for the natural variability in materials and manufacturing. By fully parameterizing the constituent materials and geometry of TPS composites, it is possible to probe all combinations of mesoscale model inputs and estimate the range of bulk material behaviors, enabling uncertainty quantification.

We focus on the development of mesoscale finite element models describing a representative volume element (RVE) consisting of a dense woven composite. We calculate volume-averaged properties commonly used in ablation models: geometric parameters such as density and fiber volume fraction, thermo-mechanical properties including thermal conductivity, specific heat, and coefficient of thermal expansion, linear elastic moduli, permeability, and tortuosity. Latin hypercube sampling (LHS) is performed to fully sample the input space capturing the natural variability in materials and uncertainty in experimental measurements. Lastly, a full regression study is performed to present the effective behavior distributions, as well as the interactions and sensitivities of input parameters revealed through the suite of calculations.

Sandia National Laboratories is a multi-mission 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-NA0003525.

**Keywords:** ablation, pyrolysis, woven composites, effective behavior, mesoscale, sensitivity analysis

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### References

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## A ready-to-use multi-fidelity gas-surface interaction module for CFD

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### Abstract

From a CFD standpoint, Gas-Surface Interaction (GSI) phenomena can be seen as a surface boundary condition to the chemically reacting Navier-Stokes equations. Solving the surface mass and energy balances at the interface by means of an external library greatly facilitates its implementation. The interface physics do not need to be treated in the CFD solver; here, the interface thermodynamic state is provided by a GSI module implemented in the MUTATION<sup>++</sup> library [1]. Both ablative and catalytic processes are considered for a broad range of fidelity levels, from elementary reactions at the material surface to local thermodynamic equilibrium conditions. A variety of other phenomena are also available, such as models for steady-state heat conduction in a solid, surface radiation and pyrolysis. Abstracting complex GSI phenomena in a library can make them easily accessible to researchers for straightforward code-to-code comparison.

The developed GSI module was coupled to an in-house CFD solver to study low-density ablators, focusing on the purely carbonaceous material Carbon Bonded Carbon Fiber (CBCF) preform by Mersen. A spherical sample of CBCF was tested in the VKI Plasmatron facility in a high enthalpy jet (Ref. [2]) for several conditions allowing us to assess its ablative properties. Two of these conditions were simulated including the processes of carbon oxidation, nitridation and sublimation. One of the main aims of the simulations was to compare a state-of-the-art elementary reactions (PSMM) model for carbon oxidation [3] with a phenomenological model [4] in order to predict the material surface temperature and recession. The results, validated with the experiments, showed that the finite-rate chemistry model provides a better insight for applications where oxidation prevails.

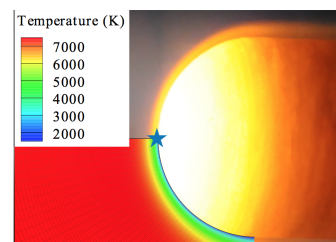
MUTATION<sup>++</sup> GSI module is openly available to the researcher and corporate communities and is currently used for applications ranging from thermal protection materials through biomass pyrolysis to meteors. In the future, the module will be available to model other types of interfaces, such as liquid - gas, and to provide the boundary conditions for material solvers as well.

**Keywords:** Ablation, Surface energy balance, Elementary Reactions Ablation

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(a) CBCF preform sample.



(b) Simulation of the plasma flow around sample.

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## Development of an Oxidation Model for Carbon Preform Ablators for use in CFD

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### Abstract

Recently, a detailed finite-rate surface chemistry model was developed for the oxidation of vitreous carbon (VC) in DSMC [1] using the molecular beam experimental data of Murray et al., [2]. The surface chemistry model consists of detailed surface reaction mechanisms such as adsorption, desorption, and several types of Langmuir-Hinshelwood (LH) reactions to characterize the oxygen-carbon interactions at the surface. This model provides excellent agreement with the experimental data for oxidation product compositions and corresponding translational energy distributions. In this work, we extend this VC model to FiberForm<sup>®</sup>, a carbon preform material used commonly as a precursor in thermal protection systems (TPS). First, in order to validate this model, we perform simulations of molecular beam scattering experiments of hyperthermal O striking FiberForm<sup>®</sup> using the Porous Media Analysis (PuMA) software [3]. The PuMA software is a suite of tools to compute effective material properties and response based on the micro-structure of the material. A detailed surface reaction framework is implemented in PuMA, in which the probabilities and the characteristic time scales of the reaction mechanisms are computed based on the reaction rate constants, sticking coefficients, surface properties, and instantaneous coverage. This framework also incorporates microscopic information regarding the detailed scattering of the products (including desorption barriers, angular scattering), in addition to the macroscopic information (reaction mechanisms, rate constants) [4]. The detailed micro-structure of FiberForm<sup>®</sup> obtained from X-ray micro-tomography is used in the PuMA simulations to capture the complexity of the porous and fibrous characteristic of FiberForm<sup>®</sup>. The VC model was applied to each fiber of the FiberForm<sup>®</sup> material, and the results of these simulations are compared to the hyperthermal beam experiments performed on FiberForm<sup>®</sup>. Figure 1 shows the experimental and numerical TOF distributions for O and CO, respectively, at 1623 K and a final angle of 45°, and their fitted IS (in the case of O), TD and slow components. The comparison of experimental and simulated angular distributions of O and CO at 1623 K is shown in Figure 2. Comparison between the experimental and DSMC time-of-flight (TOF) and angular distributions of both O and CO showed good agreement [5]. It was also found that a significantly higher amount of CO was generated when the beam interacted with FiberForm<sup>®</sup>, when compared with the vitreous carbon. This is postulated to be primarily a result of multiple collisions of oxygen with the fibers, resulting in an higher effective rate of CO production. Multiple collisions with the different fibers, resulting from the porous nature of FiberForm<sup>®</sup> was also found to thermalize the O atoms, in addition to the adsorption/desorption process. The effect of micro-structure was concluded to be very significant in determining the final composition and energy distributions of the products. Thus, an effective model for the oxygen interaction with FiberForm<sup>®</sup>, fully accounting for the detailed micro-structure, for use in Computational Fluid Dynamics (CFD) and material response codes, will be presented as part of future work.

**Keywords:** Carbon Ablation, Carbon Oxidation, Surface Chemistry, FiberForm, PuMA, Gas-Surface Interaction.

### Acknowledgements

This work was performed under the Entry System Modeling Project (Dr. M. J. Wright Project Manager) at the NASA Game Changing Development (GCD) Program and supported by NASA Grants NNX15AU92F and NNX15AD77G.

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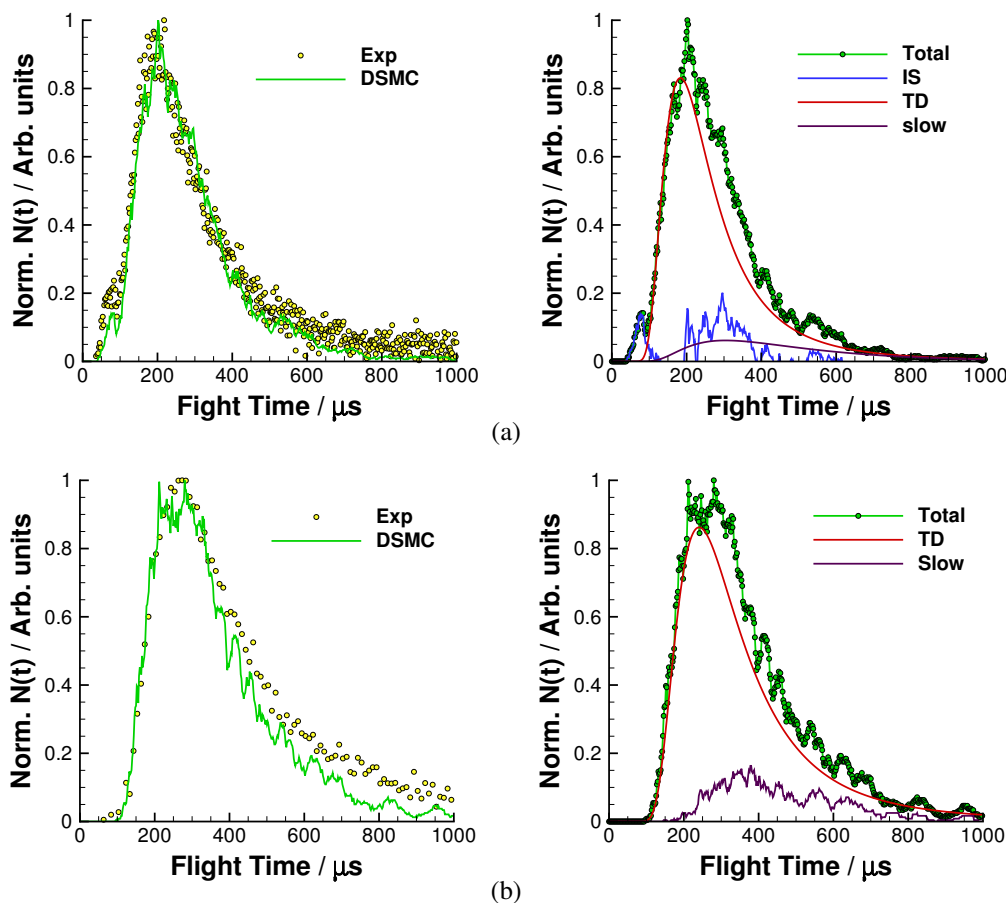


Figure 1: TOF of (a) O atom and (b) CO molecules scattering from a FiberForm<sup>®</sup> surface at incident and final angles of 45° at 1623 K. The left plot shows the comparison between the experimental and simulation results. The right plot shows the decomposition of the DSMC results into IS, TD and slow.

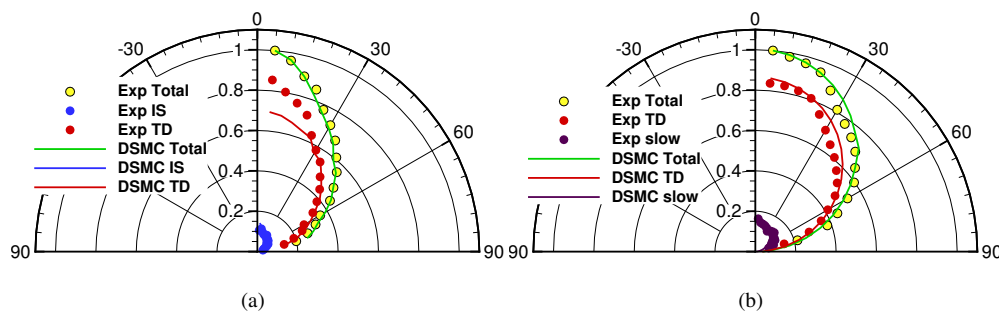


Figure 2: Comparison of experimental and DSMC results for flux integrated angular distributions of (a) O atom and (b) CO molecule scattering from a FiberForm<sup>®</sup> surface at an incident angle of 45° and final angles between 5 and 80°, at 1623 K.

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## HEEET ETU Static Point Load Tests

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### Abstract

The Engineering Test Unit (ETU) for Heatshield for Extreme Entry Environment Technology (HEEET) Project was tested at NASA Langley Research Center under static point loading conditions using different types of load heads at various interior locations. The applied static point loads were chosen to induce deflections on the ETU that correspond to deflections for a conceptual mission entry trajectory. The objectives for these tests were to evaluate the performance, and validate material properties and capabilities of the ETU in addition to obtaining detailed strain information. The ETU is a 1-meter scale, 45-degree sphere-cone, developmental heatshield which consists of three-dimensionally woven ablative thermal protection material, also referred to as HEEET, bonded to a solid composite laminate carrier substructure with a metallic support ring. The HEEET material is designed to establish capability across a wide range of missions to include Venus probes and landers, Saturn and Uranus probes, and high-speed sample return missions. Details of the ETU, static point load test setup shown in Figure 1, and test results will be presented.

**Keywords:** Three-Dimensional Woven Thermal Protection System (3-D WTPS), Material Properties, Mechanical Testing, Point Load Testing



Figure 1: ETU Static Point Load Test Setup

Abstract for 10<sup>th</sup> Ablation Workshop, September 17-18, 2018, Burlington, VT

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## HEEET ETU Thermal-Vacuum Tests

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### Abstract

The Engineering Test Unit (ETU) for Heatshield for Extreme Entry Environment Technology (HEEET) Project was tested at NASA Langley Research Center under hot and cold temperature conditions in a vacuum environment. The applied thermal cycling conditions were chosen to simulate the temperature oscillations experienced during the on-orbit/transit phase of a conceptual mission. The objectives for these tests were to evaluate the performance of the ETU in addition to obtaining detailed strain information. The ETU is a 1-meter scale, 45-degree sphere-cone, developmental heatshield constructed using three-dimensionally woven ablative thermal protection material, also referred to as HEEET, bonded to a solid composite laminate carrier substructure with a metallic support ring. The HEEET material is designed to establish capability across a wide range of missions to include Venus probes and landers, Saturn and Uranus probes, and high-speed sample return missions. Details of the ETU, thermal-vacuum test setup shown in Figure 1, and test results will be presented.

**Keywords:** Three-Dimensional Woven Thermal Protection System (3-D WTPS), Material Properties, Thermal Cycling, Thermal-Vacuum Chamber

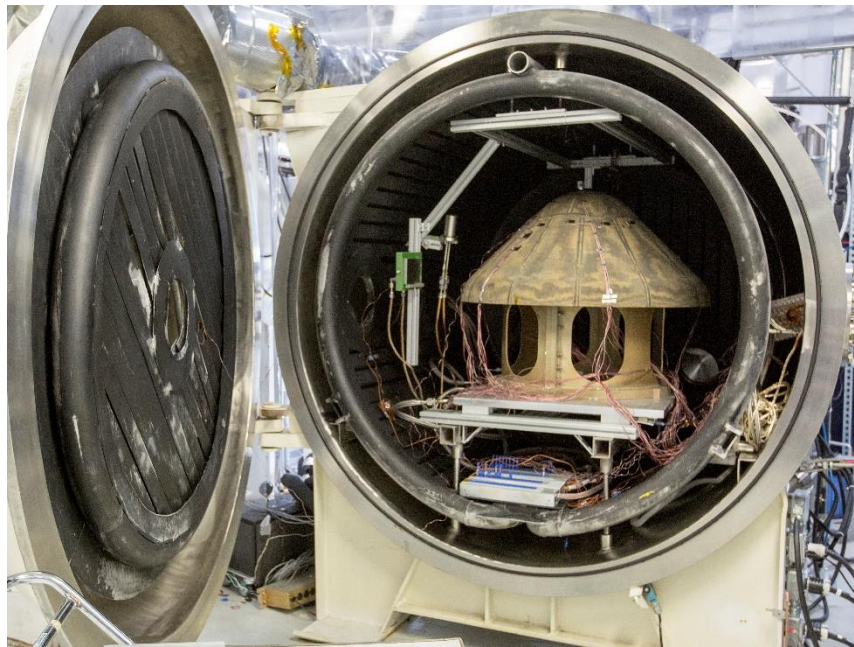


Figure 1: ETU Thermal-Vacuum Test Setup in Thermal-Vacuum Chamber

Abstract for 10<sup>th</sup> Ablation Workshop, September 17-18, 2018, Burlington, VT

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## HEEET ETU Static Pressure Tests

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### Abstract

The Engineering Test Unit (ETU) for Heatshield for Extreme Entry Environment Technology (HEEET) Project was tested at NASA Langley Research Center under a constant static pressure load at room temperature and at an elevated temperature of 250°F in an autoclave. The applied constant static pressures were chosen to simulate the static pressure distribution of a conceptual mission entry trajectory. The objectives for these tests were to evaluate the performance of the ETU in addition to obtaining detailed strain information. The ETU is a 1-meter scale, 45-degree sphere-cone, developmental heatshield constructed using three-dimensionally woven ablative thermal protection material, also referred to as HEEET, bonded to a solid composite laminate carrier substructure with a metallic support ring. The HEEET material is designed to establish capability across a wide range of missions to include Venus probes and landers, Saturn and Uranus probes, and high-speed sample return missions. Details of the ETU, static pressure test setup shown in Figure 1, and test results will be presented.

**Keywords:** Three-Dimensional Woven Thermal Protection System (3-D WTPS), Material Properties, Mechanical Testing, Autoclave

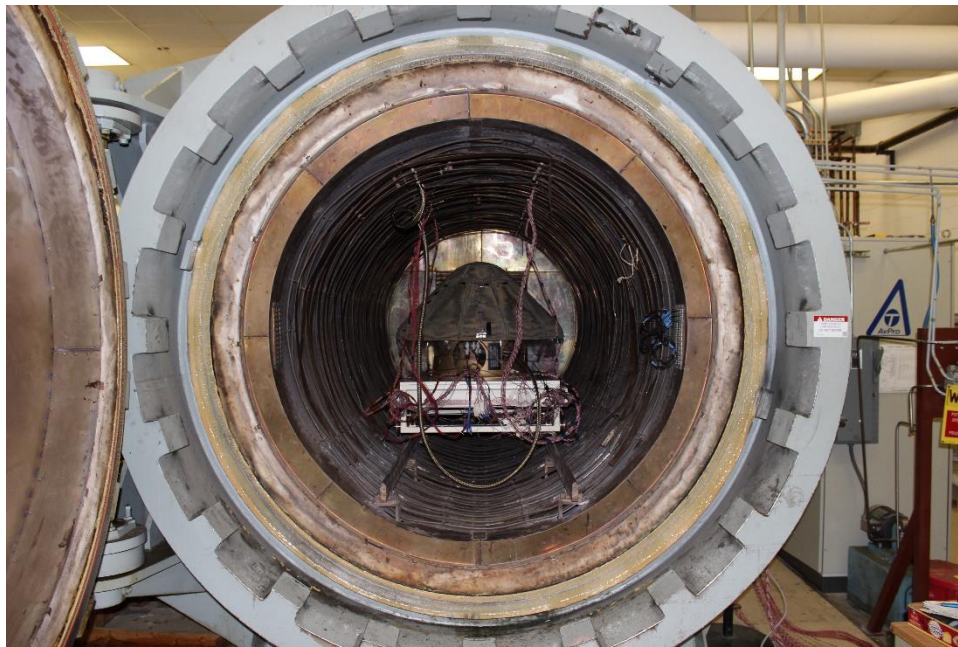


Figure 1: ETU Static Pressure Test Setup in Autoclave

Abstract for 10<sup>th</sup> Ablation Workshop, September 17-18, 2018, Burlington, VT

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# A COMPARATIVE STUDY ON ABLATION PERFORMANCE, THERMAL PROPERTIES, AND MICROSTRUCTURES OF 2D, 2.5D, and 3D CARBON/PHENOLIC ABLATIVES

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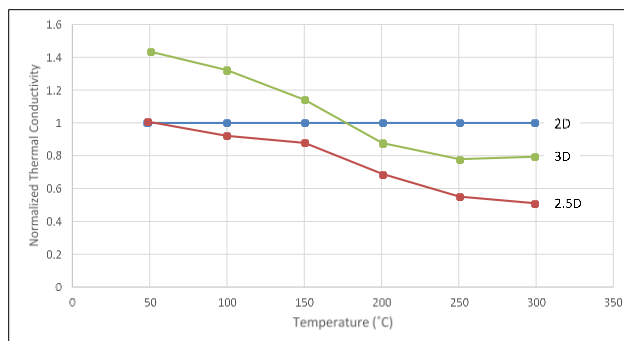
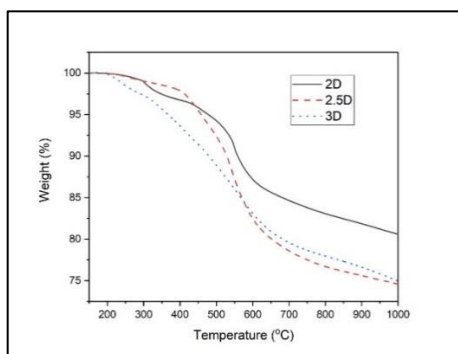
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## EXTENDED ABSTRACT

Carbon/phenolic has long been used as ablatives to protect structures from the effects of extreme environments. This study is conducted to analyze the effects of novel and existing carbon fiber architectures on ablation performance and insulative properties for three types of carbon/phenolic (C/Ph) materials. The three materials we studied are: two-, two and half-, and three-dimensional (2D, 2.5D, and 3D) C/Ph. The 2D C/Ph was manufactured by Cytec Solvay Group, the 2.5D C/Ph was manufactured by Allcomp, Inc., and the 3D C/Ph was manufactured by Ariane Group.

Analyses of the three variations of C/Ph were conducted using the following performance parameters: (a) physical property: density ( $\rho$ ); (b) thermal properties: char yield, thermal diffusivity ( $\alpha$ ), heat capacity ( $c_p$ ), and thermal conductivity ( $\lambda$ ); (c) ablation properties: depth recession percentage, recession rate, mass loss percentage, mass loss rate, peak heat-soaked temperature and time. The primary tool used to obtain ablation properties was the University of Texas (UT) oxyacetylene test bed (OTB). The OTB test results are supplemented with microstructural analyses using scanning electron microscopy (SEM).

Figure 1 shows the TGA data of the 2D, 2.5D, and 3D C/Ph at a heating rate of 20°C/min in nitrogen atmosphere and Table 1 shows the key parameters from TGA and dTGA results. The 2D C/Ph has the highest char yield (81%) and the 2.5D and 3D have similar char yield (75%).



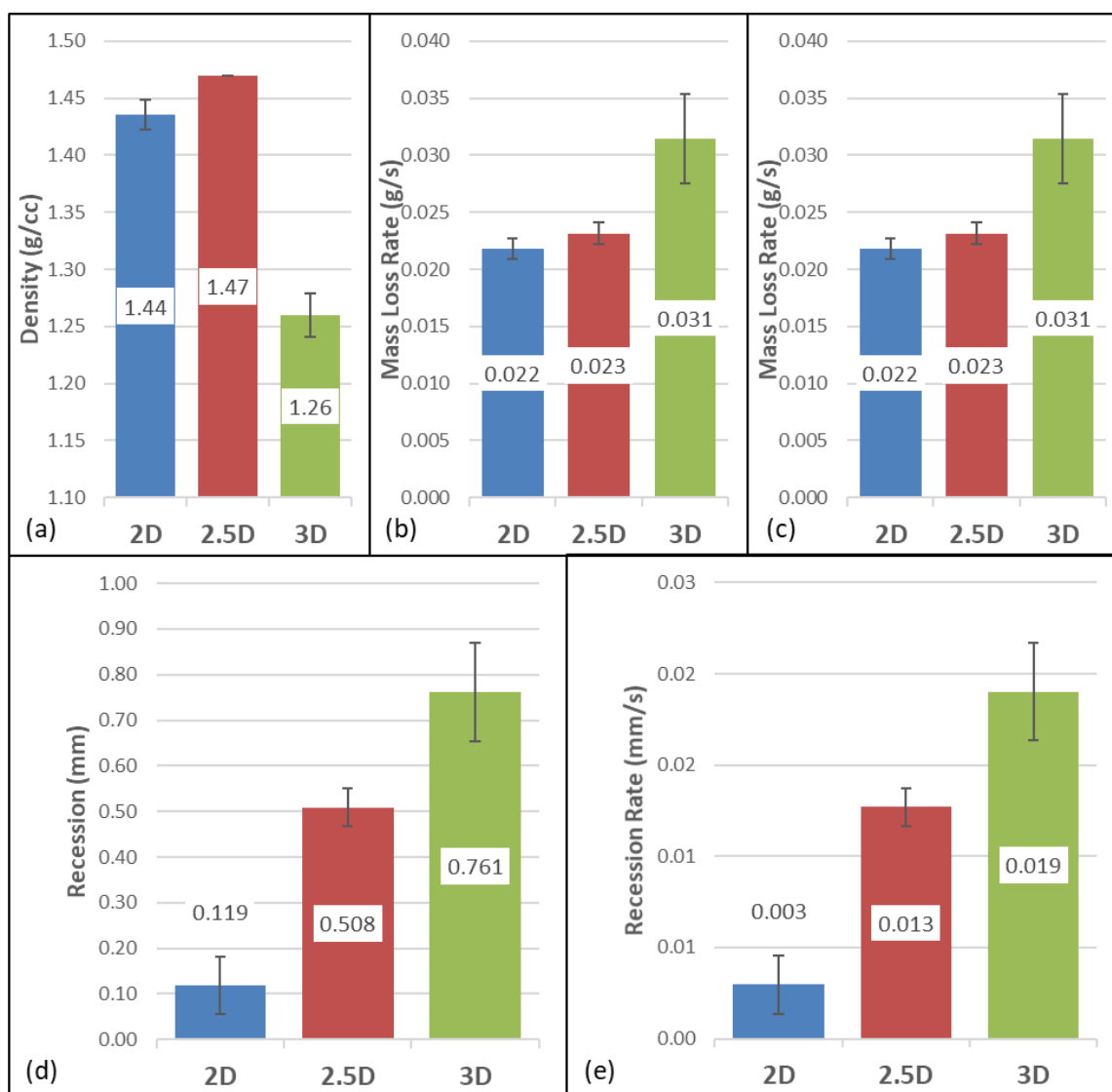
**Fig. 1.** TGA data for the three C/Ph ablatives. **Fig. 2.** Normalized thermal conductivity of the three C/Ph ablatives.

**Table 1.** Key parameter from TGA and dTGA results

Sample	Char Yield (wt%)	Peak Mass Loss Temperature (°C)
2D	80.6	548.4
2.5D	74.6	537.2
3D	75.0	563.8

Figure 2 shows the normalized thermal conductivity values of the three C/Ph ablative. The data have been normalized with respect to the 2D C/Ph results due to ITAR restrictions. The low thermal conductivity the 2.5D C/Ph shows promised as an improved alternative to the existing 2D and 3D C/Ph materials.

These C/Ph materials were analyzed on an oxyacetylene test bed (OTB) with a neutral flame, heat flux of 1,000 W/cm<sup>2</sup>, and an exposure time of 40 seconds to characterize their ablation performance. A 2.5D fiber architecture was found to have improved performance over the other tested 2D and 3D C/Ph materials due to lower surface temperature, comparable mass loss and recession, lesser thermal penetration, and lower thermal diffusivity (Fig. 3). Scanning electron microscopy analysis were used to study the pre- and post-test ablative samples to understand their material protection mechanism.



**Fig. 3.** OTB ablation test results: (a) density, (b) mass loss, (c) mass loss rate, (d) recession depth, and (e) recession rate of the three C/Ph ablative.



## Comprehensive material properties characterization of the ZURAM ablator at the VKI for material response code validation

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### Abstract

The von Karman Institute for Fluid Dynamics (VKI) is currently carrying out an intensive effort to assess the state-of-the-art modeling and prediction of ablative thermal protection materials in Europe. In this framework, the ZURAM ablative material developed by the German Aerospace Center (DLR) will be experimentally characterized on two different levels: detailed thermal analysis and plasma testing, in order to provide an extensive database for inclusion in material response codes. The distribution of the ZURAM data is not restricted, allowing for the dissemination of the data, obtained results (and the actual material) within the research community.

ZURAM has been preliminarily studied by DLR [2], however, many properties are still unknown or present large uncertainties and depend on the batch of ZURAM produced. The detailed thermal analysis (TGA/DSC, LFA) will provide code input parameters such as pyrolysis kinetic rates, heat capacity, and thermal diffusivity (Fig 1.a).

The ablation tests performed in the VKI Plasmatron facility will allow the in-situ measurement of emissivity, the surface and pyrolysis recession rates, as well as the temperature evolution on the surface and inside the test samples at different pressures, test enthalpies, and test gases (Fig 1.b and 1.c).

Following the experimental characterization, our goal is to use different European material response codes for their inter-comparison and comparison with the experimental data. This will allow the development of an open material database and new test cases, which will be shared with the community for code verification and validation.

**Keywords:** carbon/phenolic ablator, thermal analysis, material characterization, code development

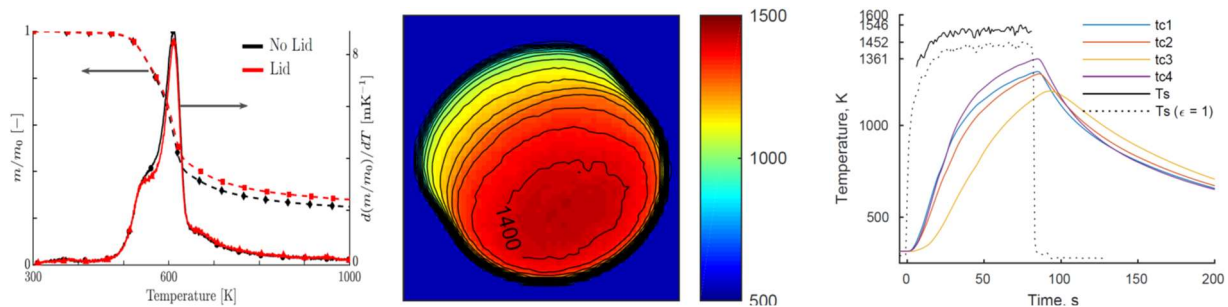


Figure 1: TGA & DTGA curves for niaouli showing the final char content, ZURAM infrared thermography image during test (middle), and surface and internal temperature histories (right).

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# Nitridation and Surface Catalyzed Recombination on High-Temperature Carbonaceous Fiber Materials

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## Abstract

In January, 2006 the Stardust capsule brought material from a comet back to earth re-entering the atmosphere on a ballistic trajectory at the highest speed recorded to date,  $\sim 15$  km/s [1, 2]. The heat-shield, made of PICA, survived re-entry and was thus available for post-flight inspection. Attempts to simulate the aero-thermal heating of re-entry in ground test showed that the computed heat transfer rate could not account for the measured recession unless nitrogen atom recombination on the surface ( $N+N+[s] \rightarrow N_2+[s]$ ) was included at the maximum possible rate [3]. Early laboratory measurements have shown that nitrogen recombination is relatively inefficient, compared to oxygen [4]. A more recent investigation of these reactions was undertaken in partnership with SRI International, who made measurements of the carbon nitridation rate ( $C_{[s]}+N \rightarrow CN$ ) of high-purity POCO graphite in their diffusion sidearm reactor [5]. Their measured nitridation efficiency ranged from  $0.2(10)^{-3}$  to  $9.8(10)^{-3}$ , depending on sample temperature (up to  $\sim 1300$  K), and these values compared reasonably well with UVM measured efficiency of  $6.45(10)^{-3}$  [6]. No evidence of surface-catalyzed recombination of atomic nitrogen to form diatomic nitrogen was found in the SRI experiments. However, measurements of nitrogen recombination on higher-temperature ( $\sim 1800$  K) POCO graphite at the University of Vermont (UVM) suggest that nitrogen recombination is highly efficient [7], supporting the modeling assumption. Previous work in our laboratory provided quantitative measurements of both the nitridation and surface catalyzed recombination rates on high-purity graphite. The nitridation rate was  $2.51 \pm 0.44$  m/s, while the recombination rate was  $57.2 \pm 14.9$  m/s [6]. It is the recombination rate that is responsible for the high surface temperatures seen on graphite in our ICP torch facility tests.

The discrepancy between SRI and UVM results suggests that there is some unknown value of graphite surface temperature below which nitrogen recombination does not proceed and this warrants further investigation. Owing to this, an effort at UVM has begun to investigate carbon nitridation and nitrogen recombination on fibrous carbon materials (such as those comprising the substrate of PICA, or on PICA char surfaces) exposed to nitrogen and argon-buffered nitrogen plasmas in the UVM 30 kW ICP Torch Facility. This effort aims not only to measure the specie gradients of N atom within the chemically reacting boundary layer (via planar TALIF illustrated in Figure 1 right side) but also gradients of other key species in the carbon-nitrogen system including C atom (via 2-photon LIF), CN radical (via emission spectroscopy as seen in right side of Figure 1), and  $N_2$  molecule (via vibrational Raman as seen in left side of Figure 2 and pure rotational Raman as seen in right side of Figure 2). This talk will highlight past progress on the matter at UVM, current status of the effort, and where the work will be heading in the near term.

*Keywords:* Nitridation, Gas Surface Interaction, Catalysis

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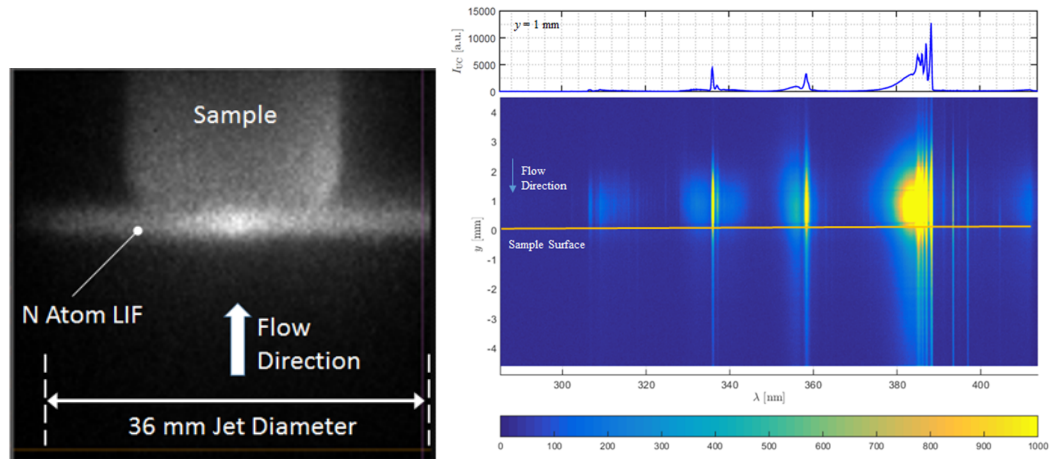


Figure 1: (Left) N atom LIF above a POCO graphite surface in an N<sub>2</sub> plasma, (Right) Spatially resolve emission spectra of CN above a POCO graphite surface in an N<sub>2</sub> plasma.

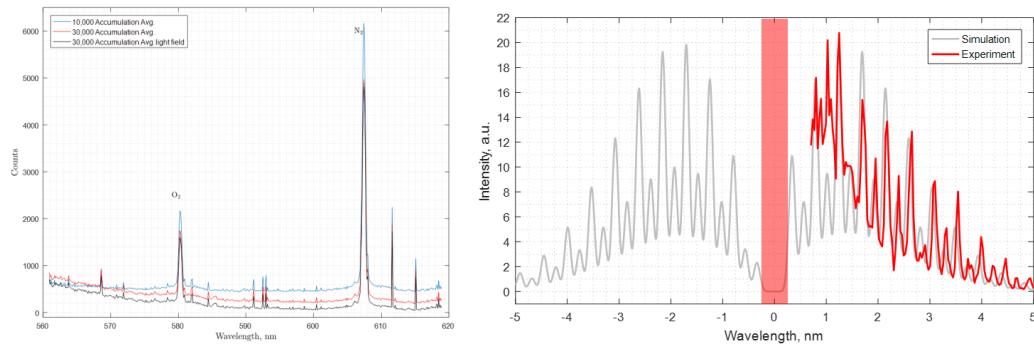


Figure 2: Vibrational Raman of O<sub>2</sub> and N<sub>2</sub> in atmospheric air (Left) and pure rotational Raman of N<sub>2</sub> taken in the ICP test cabin with cold N<sub>2</sub> flow (Right). Both acquired from scattering of incident 532 nm light.

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doi: 10.2514/6.2013-924

## Development of a low-mach number flow solver for the UVM ICP torch

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### Abstract

A numerical model has been developed for the 30 kW inductively coupled plasma torch facility at the University of Vermont which couples finite rate chemical kinetics and high temperature thermodynamic and transport properties with a computational fluid dynamics flow solver. Physics-based surface boundary conditions for wall temperature and catalytic efficiency were implemented to represent the different test article materials used in the experimental facility. Simulations were performed for an oxygen-argon plasma in order to validate the models developed in this work by comparison to experimentally-obtained data for temperature and species populations in the thermal boundary layers above copper, cold quartz, and hot quartz test articles. Good agreement between measured and computed data is observed.

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## Towards the prediction of the Mars 2020 heatshield material response

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### Abstract

NASA's next mission to Mars, the Mars 2020, will use the spare heatshield of the Mars Science Laboratory (MSL) for thermal protection during entry, descent and landing. The heatshield is a tiled system made of PICA (Phenolic Impregnated Carbon Ablators) blocks. In this work, we discuss progress towards predictive modeling of PICA ablation using the Porous-material Analysis Toolbox based on OpenFOAM (PATO) software [1,2]. In PATO, ablation of low-density carbon-phenolic ablators is modeled by solving the conservation equations of solid mass, gas mass, gas momentum and total energy, using a volume-averaged formulation that includes production of gases from the decomposition of the polymeric matrix. The aerothermal environment at various Knudsen regimes is fed to PATO as surface boundary conditions. In the rarified regime, the environment around the MSL aeroshell is computed using the Direct Simulation Monte Carlo code SPARTA [3], while in the continuum regime the CFD code Data Parallel Line Relaxation (DPLR) [4] is used. The radiation heating from the environment is added to the surface energy balance by computing radiative flux at Mars entry conditions using the Nonequilibrium air radiation (NEQAIR) program [5]. Effective material properties for PICA are obtained through a combination of experiments and predictive simulation using the Porous Microstructure Analysis (PuMA) software [6]. In preparation to Mars 2020 post-flight analysis, the predictive material response capability is benchmarked against flight data from the MSL Entry, Descent, & Landing Instrument (MEDLI).

**Keywords:** Mars Science Laboratory, Heatshield, Porous media, Equilibrium chemistry, Ablation, Pyrolysis

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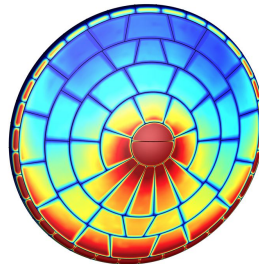


Figure 1: Material response of a full-scale tiled heatshield using PATO software.

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## Recent developments to the Porous Microstructure Analysis (PuMA) software.

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### Abstract

The Porous Microstructure Analysis (PuMA) software [1] is a suite of tools for the analysis of porous materials and generation of material microstructures. From microstructural data, often obtained through X-ray microtomography [2], PuMA can determine a number of effective material properties and perform material response simulations. Version 2.2 includes capabilities for computing volume fractions, porosity, specific surface area, effective thermal and electrical conductivities, and continuum and rarefied diffusive tortuosity. PuMA can also simulate competitive diffusion/reaction processes at the micro-scale, such as surface oxidation.

In this poster, recent advancements to the PuMA software are detailed. The refactoring of PuMA into V3.0 is described, including the highly modular design and PuMA Testing Framework (PuMATest). A 3D, fully parallel numerical scheme for computing the effective thermal conductivity of anisotropic materials was implemented, based on the Multipoint Flux-Approximation method [3]. The numerical method enables simulations of thermal transport in woven and fibrous materials with anisotropic local thermal conductivity. A particle-based solver for simulating molecular beam-surface scattering experiments [4] was implemented and parallelized within PuMA. The solver can simulate the high speed gas transport and complex surface reaction mechanisms. Since particle-particle collisions are negligible in the specific experimental setup, the PuMA implementation provides a substantial speed increase over DSMC simulations of molecular beam experiments. The PuMA module will be used to develop finite-rate surface chemistry models for fibrous carbon ablators.

Additional new capabilities in version 3.0 of the software include 3D image filtering algorithms; simple mean and median filters as well as edge-preserving techniques were implemented. Advanced material generation capabilities have been implemented, including the generation of complex 2D and 3D woven structures, curved fibers, multiple cross-sectional designs, and fiber clustering. Particular effort was invested in optimizing the computational efficiency and parallelization of the new capabilities. Finally, PuMA V3.0 was coupled with the Dakota software [5] to conduct uncertainty quantification, calibration, sensitivity analysis, and optimization for microscale simulations.

**Keywords:** X-ray Microtomography, Heat Transfer, Diffusion

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## CFD modeling of subsonic plasma flow for ablation experiments

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### Abstract

We simulate subsonic plasma flows over a fully catalytic cylindrical probe using US3D, a state of the art parallel CFD software developed at the University of Minnesota[1, 2]. The flow conditions are based on the ablation experiments carried out at the Von Karman Institute for Fluid Dynamics (VKI)[3]. The flow is in thermal equilibrium at the inlet and the inlet species mass fractions and enthalpy are calculated using the NASA Chemical Equilibrium Analysis (CEA) database by specifying inlet temperature and pressure. The simulations use modified Steger-Warming flux vector splitting with second-order accuracy for the treatment of convective fluxes. Viscous fluxes are computed using weighted least-square reconstruction of the gradients. Blottner curve fits for viscosity, Eucken relation for thermal conductivity and a single diffusion coefficient based on a Lewis number of 1.4 are used. Park's two temperature non-equilibrium chemistry model for 11-species air is used for chemical reaction with one temperature used for translational/rotational modes and the other temperature for vibrational and electronic modes as described by Norman *et al.*[4]. The rates of reverse reactions are found using detailed balance and vibrational relaxation is modeled using Millikan and White correlation. The axisymmetric grid contains approximately 30,000 cells, with the distance from wall-adjacent cell centers to the wall of 5  $\mu\text{m}$ . Further refinement of the grid did not change the heat flux on the probe wall significantly.

In each case the inlet conditions are adjusted until we match the experimentally measured cold wall heat flux at the stagnation point. We simulated 9 cases in total and show the results for an example simulation case here. The inlet is a subsonic plasma (velocity = 360 m/s) in equilibrium at 6000 K and 1715 Pa. The probe is a fully catalytic isothermal wall at 350 K. The outlet pressure is maintained at 1700 Pa. Figure 1 shows the contours of x-velocity with streamlines superposed. Flow deceleration as it approaches the probe and boundary layer growth are evident. Figure 2 shows the heat flux along the probe as a function of distance from the stagnation point. The simulation stagnation point heat flux ( $1.00 \text{ MW/m}^2$ ) is approximately 2.1% less than the experimentally measured cold wall heat flux ( $1.021 \text{ MW/m}^2$ ). As shown in Fig. 3, the simulation boundary layer edge enthalpy (28.4 MJ/kg) is close to the boundary layer edge enthalpy extracted from the experimental data (22.7 MJ/kg) using the Local Heat Transfer Simulation (LHTS) method[3]. Further research will investigate the models and assumptions used by the LHTS method compared to US3D to understand the differences in the boundary layer edge enthalpy. As seen in Fig. 4, the boundary layer edge is not in thermal equilibrium. The goal of this work is to properly characterize the freestream using US3D to simulate stagnation point and off-stagnation point ablation and compare it to experimental data.

**Keywords:** Subsonic Plasmas, Simulation

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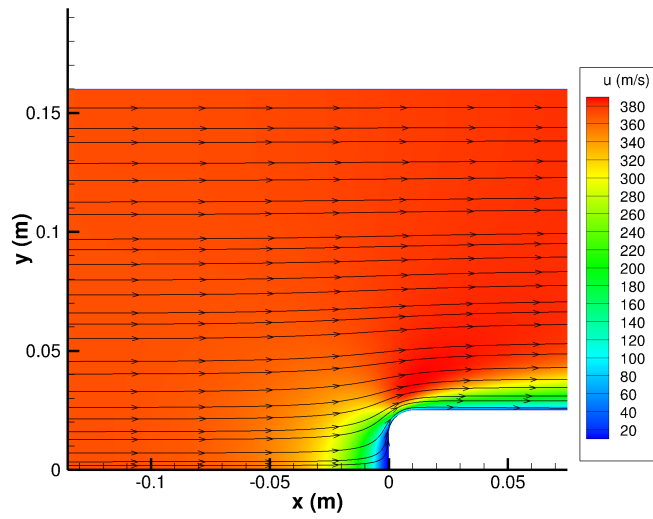


Figure 1: Contours of x-velocity with streamlines superposed.

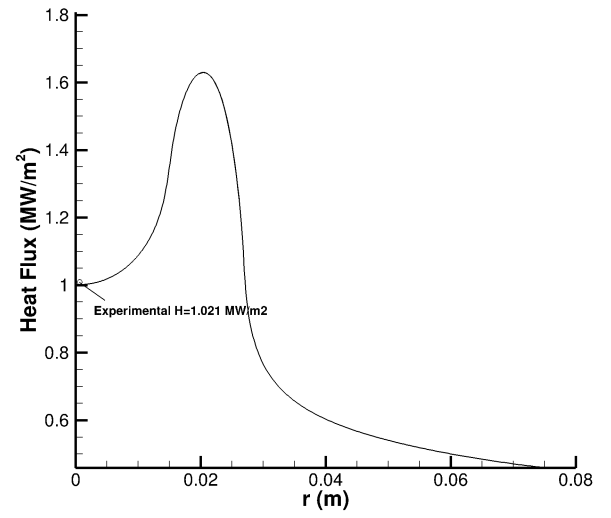


Figure 2: Heat flux along the probe as a function of the distance from the stagnation point.

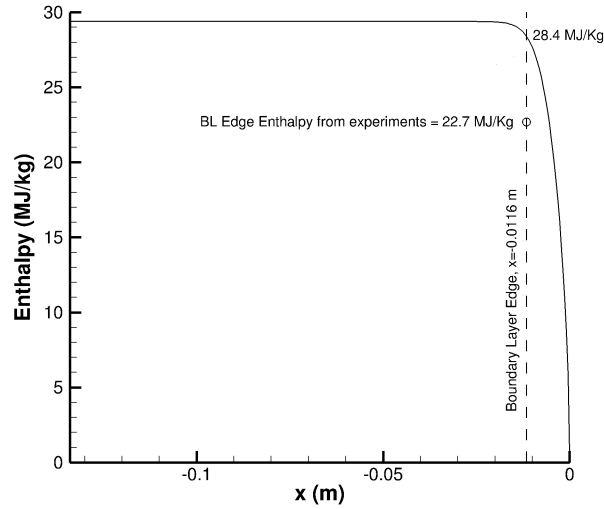


Figure 3: Enthalpy variation along the stagnation line.

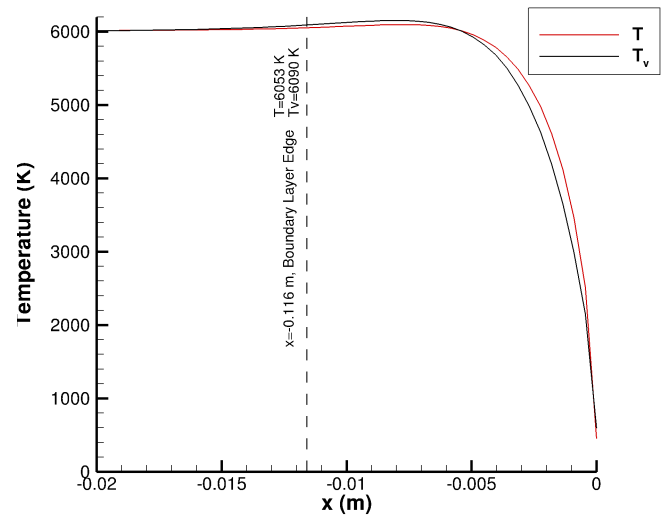


Figure 4: Temperature along the stagnation line near the stagnation point.

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## Computing Surface Properties on Thermal Protection System Microstructure

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### Abstract

In atmospheric reentry missions, ablative carbon-based thermal protection systems (TPS) are used to mitigate the heat loads acting on the vehicle. They are often classified as porous or nonporous carbon ablators consisting of fibrous microstructures. During the ablation process, the thermal stresses and traction forces acting on the TPS microstructure, combined with its oxidation, could affect its structural integrity. Hence, it is important to have the capability to model the thermo-structural response of a TPS structure. While CFD is capable of predicting the overall stress and heat flux acting on TPS surfaces at a macroscopic level, the direct simulation Monte Carlo (DSMC) method can study these effects on the TPS microstructure at a microscopic level. The capability of DSMC to resolve microscales and the ability of the cut-cell algorithm in the parallel Molecular Gas Dynamics Simulator (MGDS) developed at University of Minnesota [1, 2, 3] to deal with complex geometries make it possible to simulate flows over the cracks, crevices and protruding granules of real samples. [4].

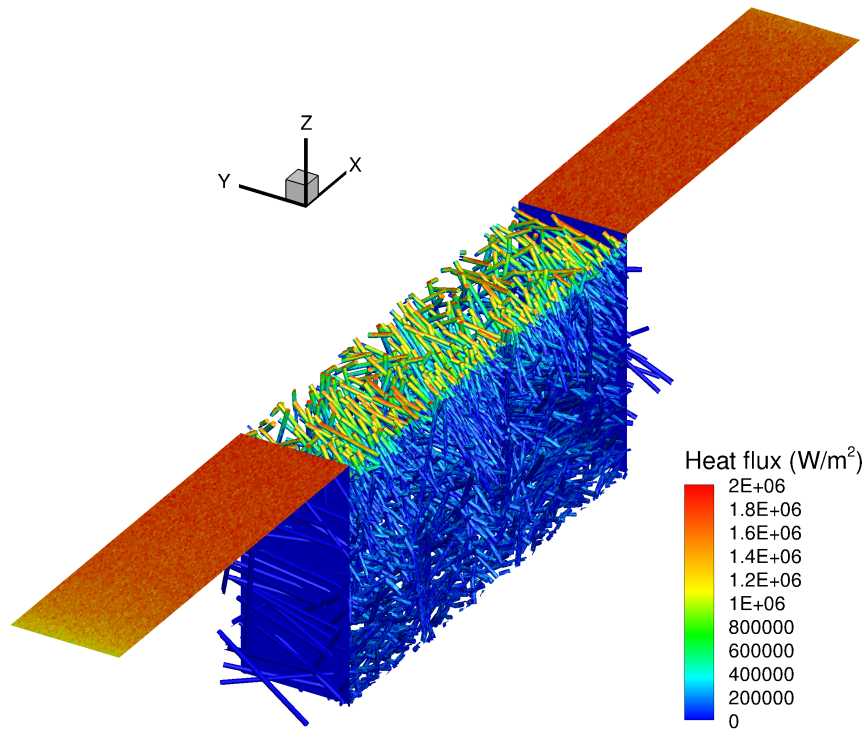


Figure 1: Heat flux ( $W/m^2$ ) acting on TPS microstructure

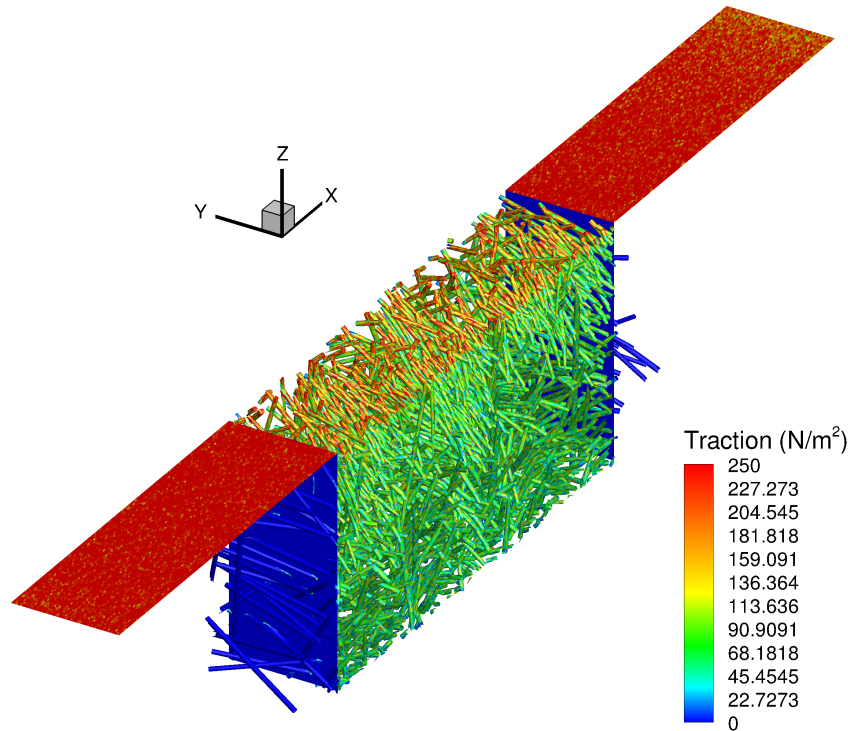


Figure 2: Traction force per unit area ( $N/m^2$ ) acting on TPS microstructure

We use DSMC simulations to model relevant boundary layer flows over realistic microstructures [5] that can capture all nonequilibrium physical processes including diffusion, convection, heat flux, surface chemistry, and even pyrolysis blowing of the gases during ablation. Figures 1 and 2 show the heat flux and traction force respectively, acting on a realistic TPS microstructure, estimated from a DSMC simulation of a hypersonic boundary layer flow over the TPS, using profiles extracted from the results of a CFD simulation [6] of the Stardust entry at 68.9 km altitude. Traction force per unit area ( $N/m^2$ ) acting on the surface is defined as the magnitude of the total force acting on it in the non-normal direction. The focus of the present work is to simulate hypersonic boundary layer flow over TPS microstructures and to analyze the effect of the resulting heat flux and traction acting on the structure.

**Keywords:** Thermal Protection System, Heat transfer, Fiber Microstructure, Thermal stress, Traction forces

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# Competing reaction pyrolysis model applied to carbon/phenolic ablators

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## Abstract

A polymeric material exposed to high temperatures decomposes into a carbonaceous char and releases gaseous products. This process is known as pyrolysis. Thermal decomposition via pyrolysis is usually modeled using combinations of Arrhenius-type equations.

Traditional models for heat shield materials adopted in aerospace applications use a set of parallel reactions to model the pyrolysis of the phenolic resin. This is the case of state-of-the-art ablator codes for carbon/phenolic materials, such as those used to simulate the response of NASA's Phenolic Impregnated Carbon Ablator (PICA) [1]. In this classical approach, a solid is assumed to be made up of different solid phases that independently undergo a single pyrolysis reaction with a predefined mass loss [1]. Independent reaction schemes allow to accurately reproduce experimental results only in a restricted range of conditions (e.g. at a single heating rate). Nevertheless, they fail to predict the decomposition at high heating rates where the polymeric phase pyrolyzes following different reaction pathways [2].

Here, we develop a new approach to model the decomposition of phenolic resin based on competing reactions. This approach follows well established techniques used in biomass pyrolysis research [3]. In a competing reaction scheme, a solid decomposes following simultaneously different kinetic pathways and, depending on the heating rate, selected paths are favored over others. It is expected that this approach will enable modeling decomposition of phenolic at heating rates experienced during flight, a notable leap in the current simulation capabilities for PICA-like ablators.

**Keywords:** carbon/phenolic ablator, pyrolysis, competing reactions, modeling

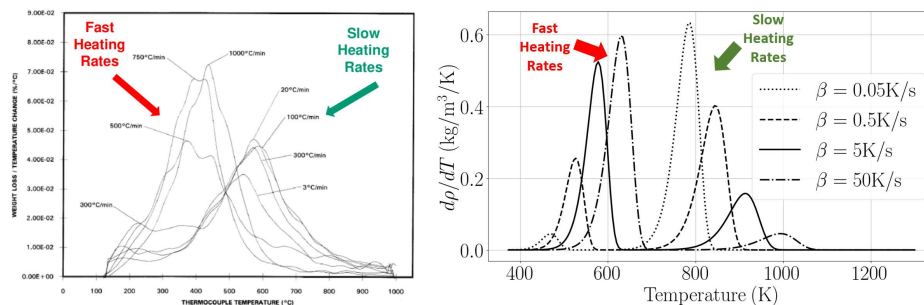


Figure 1: Experimental measurements of phenolic resin pyrolysis at largely varying heating rates [2] (left). Preliminary computations of density variations using the competing reaction scheme show a similar trend of that observed in the experiments (right).

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# Material Response Analysis of a Titan Entry Heatshield

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## Abstract

Accurate calculation of thermal protection material response is critical to the vehicle design for missions to the Saturn moon Titan, such as the proposed Dragonfly mission. In this study, Icarus [1], a three-dimensional, unstructured, finite volume material response solver under active development at NASA Ames research center, is used to compute the in-depth material response of the Huygens spacecraft along its Titan entry trajectory [2]. The heatshield analyzed in this study consists of a five-layer stack-up of PICA[3], aluminum honeycomb, adhesive, and face sheet materials. During planetary entry, the PICA outer layer is expected to receive a large enough heat pulse for the material to undergo pyrolysis. A surface energy balance boundary condition that captures both the time- and spatial-variance of surface heating rate during entry is used in the simulation. The input surface convective heating rates and pressures were computed using the DPLR CFD code[4].

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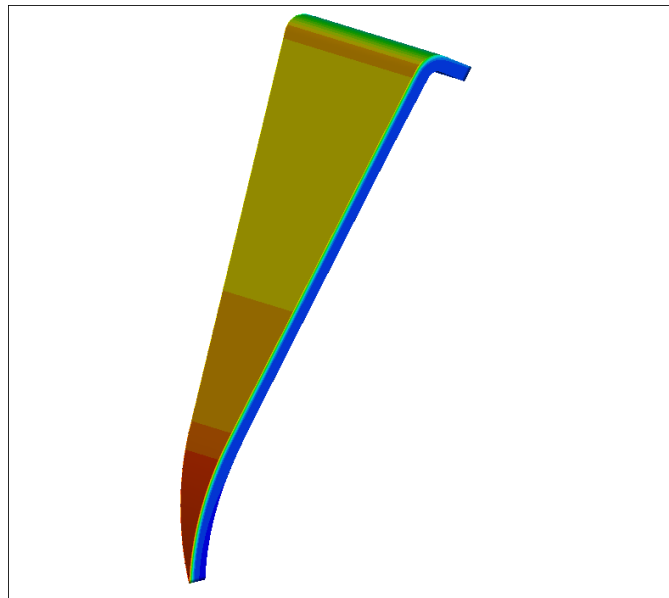


Figure 1: Temperature contours of a Titan entry vehicle heatshield.

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## Significance of DSMC computed aerothermal environments in the rarefied regime for atmospheric entry material response

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### Abstract

During Mars atmospheric entry, the Mars Science Laboratory (MSL) was protected by a 4.5 meters diameter ablative heatshield assembled in 113 tiles [1]. The heatshield was made of NASA's flagship ablative material, the Phenolic Impregnated Carbon Ablator (PICA) [2]. The Porous material Analysis Toolbox based on OpenFOAM (PATO) [3, 4] is used for the material response part of this study. The governing equations are volume-averaged forms of solid mass, gas mass, gas momentum and total energy conservation, including pyrolysis gas production. The boundary conditions at the heatshield front surface are interpolated in time and space from the aerothermal environment at discrete points of the MSL trajectory [5]. The objective of this work is to study the impact of computing the aerothermal environments in the rarefied regime using the direct simulation Monte Carlo (DSMC) on the material response. The DSMC code SPARTA [6] will be used to compute environments prior to 48.4 s of entry where the Knudsen number is such that the Navier-Stokes equations can be inaccurate. As an extension to previous work, the CFD software Data Parallel Line Relaxation (DPLR) [7] will be used to compute the hypersonic environments for a fully turbulent boundary layer assumption from 48.4 s up to 100 s of entry along the MSL 06-05 99.87% heat load trajectory.

**Keywords:** Mars Science Laboratory, DSMC, CFD, Material Response, TPS.

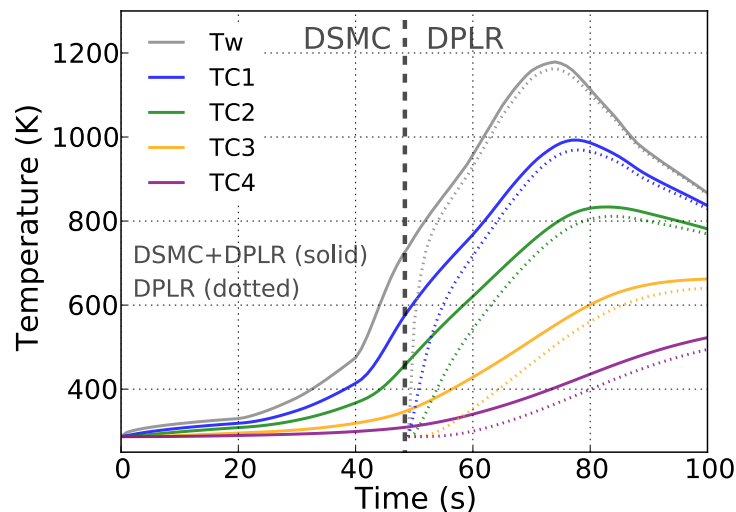


Figure 1: PATO surface and in-depth thermal response at MISP4, using DPLR only and DSMC+DPLR aerothermal environments.

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# A Chemical Equilibrium Approach to Silicon Carbide Oxidation

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## Abstract

Ultra-High Temperature Ceramic (UHTC) materials, including silicon carbide (SiC), are of interest in hypersonic aerospace applications due to their refractory nature and oxidation resistance. A macroscopic, thermodynamic chemical equilibrium approach is developed and investigated for SiC oxidation. This approach utilizes an open-system mass balance, accounting for boundary layer diffusion and equilibrium between gas-phase and condensed surface species. Active-passive and passive-active oxidation transition conditions predicted with this approach are compared to existing theories based on Wagner's model for boundary layer diffusion [1], as well as experimental data in oxygen and air [2][3]. Predicted oxygen transition pressures bound the range of available data within an order of magnitude. Applications to surface-energy-balance and surface-mass-balance calculations are examined, and active oxidation rates agree with experimental oxidation kinetics within a factor of 2-3 across a temperature range from 1800K to 2500K [4]. A thermodynamic "hysteresis" is hypothesized for both passive-active and active-passive transitions. The model is then applied to a 1-D material response test case, and a surface temperature jump [5] is demonstrated for pure SiC undergoing passive-active transition in an aerothermal heating environment.

**Keywords:** UHTC, Silicon carbide, Oxidation, Modeling, Material response

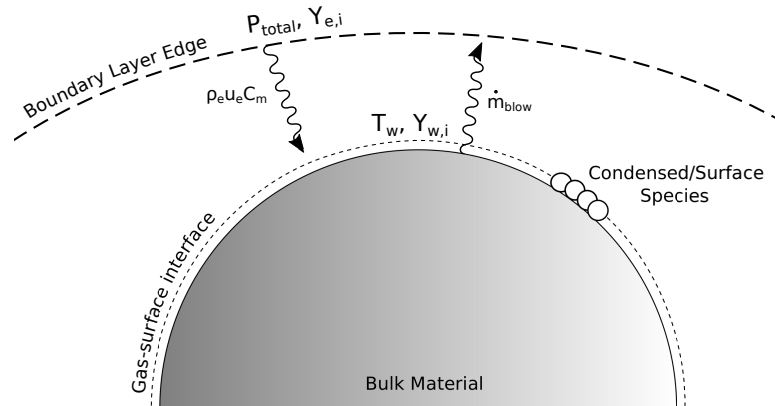


Figure 1: Open system surface mass balance. Three regions are present: the boundary layer edge, the gas-surface interface, and the bulk material.

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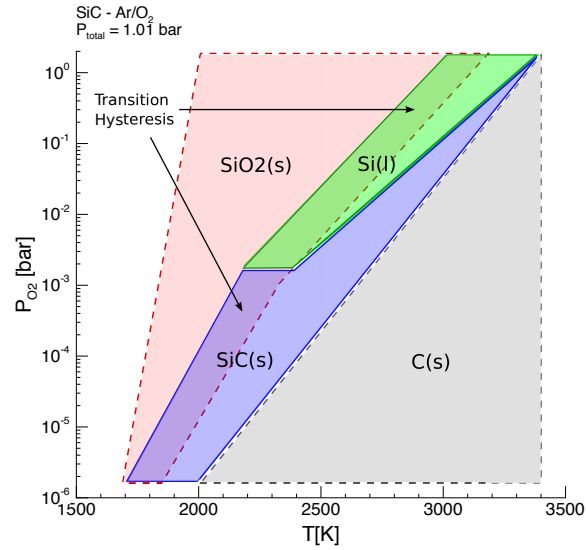


Figure 2: Surface phase diagram for SiC-Ar/O<sub>2</sub> system, (s) denotes solid phase, (l) liquid phase.

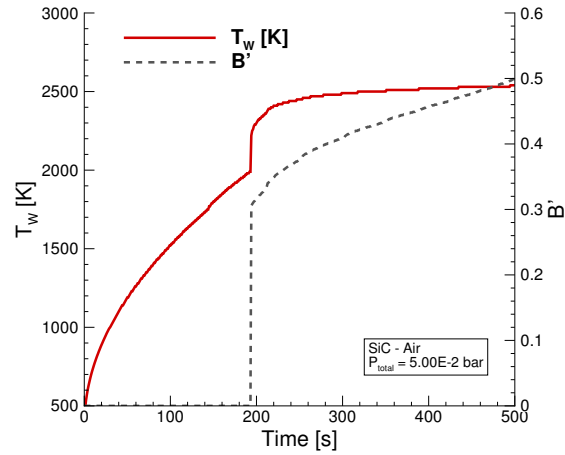


Figure 3: Surface temperature vs. time for MTA-12 conditions [5] over 0.1m 1-D domain.

## Kentucky Re-entry Universal Payload System (KRUPS): Sub-orbital Flights

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### Abstract

KRUPS (Kentucky Re-entry Universal Payload System) is an adaptable test bed for re-entry science experiments, with an initial application to Thermal Protection Systems (TPS). Because of the uniqueness of atmospheric entry conditions that ground testing is unable to replicate, scientists principally rely on numerical models for predicting entry conditions. The KRUPS spacecraft, developed at the University of Kentucky, provides an inexpensive means of obtaining validation data to verify and improve these models. To increase the technology readiness level (TRL) of the spacecraft, two sub-orbital missions were developed. The first, KUDOS, was a sub-scale prototype that launched aboard a Terrier Improved Malamute rocket to an altitude of 150 km. The second, KOREVET, was the full-scale system that launched under similar conditions and improved on the previous mission's shortcomings and aimed to collect and transmit re-entry data through Iridium. A TRL of 5 was achieved and maintained throughout these missions and improvements are currently underway, mainly in communications, to ultimately launch multiple capsules from the ISS.

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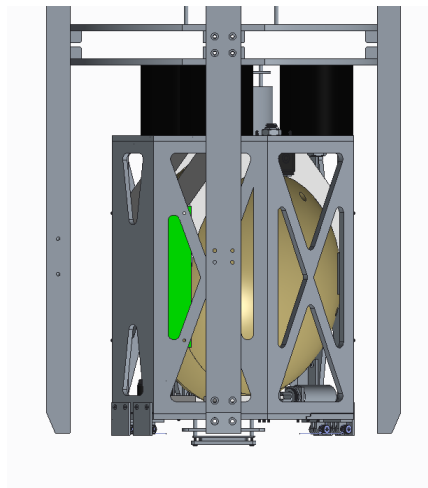


Figure 1: KOREVET CAD layout

# Numerical reconstruction of spalled particle trajectories in an arc-jet environment

Raghava S. C. Davuluri<sup>a,\*</sup>, Kaveh A. Tagavi<sup>a</sup>, Alexandre Martin<sup>a</sup>

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## Abstract

Spallation, a form of thermo-mechanical ablation, is defined as a mass removal mechanism of the material in the form of particle ejections into the flow field when subjected to intense heat. The presence of spalled particles in the flow field affects the surface heating rates. The interactions of the particles chemically with the gas lead to modification of the flow field. Furthermore, the ejections also accelerate the material recessions and thus, the performance of the ablator.

To quantify and qualify the behavior of ejected particles, experiments were conducted at NASA Langley's HYMETs arc-jet facility [1]. High-speed imagery and particle tracking velocimetry analysis were used to obtain the trajectories and their kinematic information. However, the size and other ejection parameters of the particles were not possible to be determined through direct measurements. It is important to know that the initial state of the spalled particles to have a better understanding of how the particles are formed, and what process leads to their sudden ejection. To achieve this, a hypersonic flow field solution is computed, based on the sample geometry and test conditions, using Kentucky Aerodynamic and Thermal-response Solver (KATS) [2]. A *validated* lagrangian particle-tracking code [3], developed at the University of Kentucky, is used to determine the initial size and other ejection parameters of particles whose trajectories were identified.

**Keywords:** Spallation, Ablation, Arcjet, Thermal protection system

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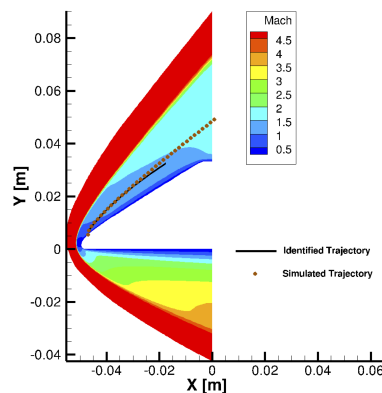


Figure 1: Reconstructed Numerical Trajectory

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## DSMC Simulation of Flow Through Various TPS Microstructures

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### Abstract

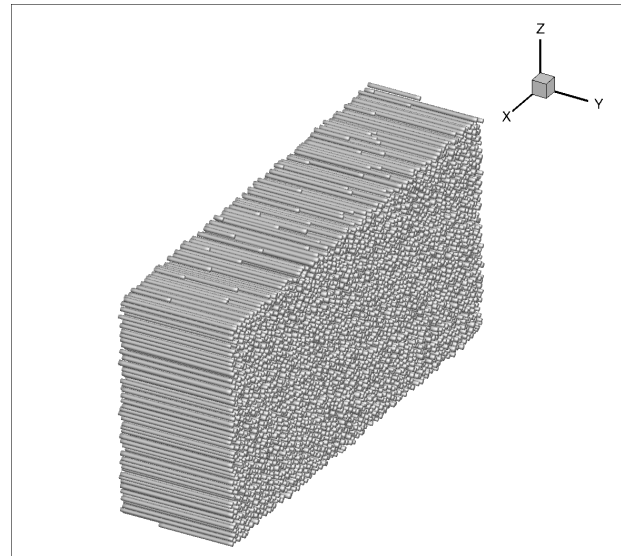
The overall objective of the current project is to improve the predictive modeling of the chemical and structural failure of porous ablative materials. The project consists of using the DSMC method to simulate boundary layer flow over resolved microstructures at flight relevant conditions. The main aim of this work is to examine the post-processing of surface properties on select fibers. FiberGen is used to generate different fiber bundles and has the capability of generating an array of fibers where the user can control the distributions of three-dimensional orientations, fiber diameters, and material characteristics such as bulk porosity [1]. Each fiber is modeled as a cylinder and is made up of many elements which is in turn made up of many triangles. The code keeps track of each fiber property including a distinctive ID number, radius, centroid in the x,y, and z direction, and the polar and azimuthal angles. One aim of this work is to link these fiber properties (in the fiber generation process) with the post-processed DSMC simulation results. This will allow a direct association of fiber properties; for example one could extract fibers whose centroid is within the first tenth of a millimeter of the surface. In addition, properties including the local heat flux as well as the thermal and structural stress fields on fibers are important. Due to the three dimensional complexity, it is particularly useful to analyze groups of fibers based on their surface properties. This work will simulate boundary layer flow over various fiber bundle configurations, as shown in Figure 1, and subsequently post-process surface properties on individual fibers. Based on a created fiber bundle, one is able to associate which fiber belongs to which set of STL triangles thereby allowing one to post-process individual fibers of interest. Enhancing the post-processing capability of individual microstructure properties will make it easier to isolate fibers of interest and to examine the heat flux, shear stress, gas-surface interactions, and fiber response in a variety of ways; both individually and averaged.

**Keywords:** Ablation, Material Response, Boundary-Layer Flow, DSMC

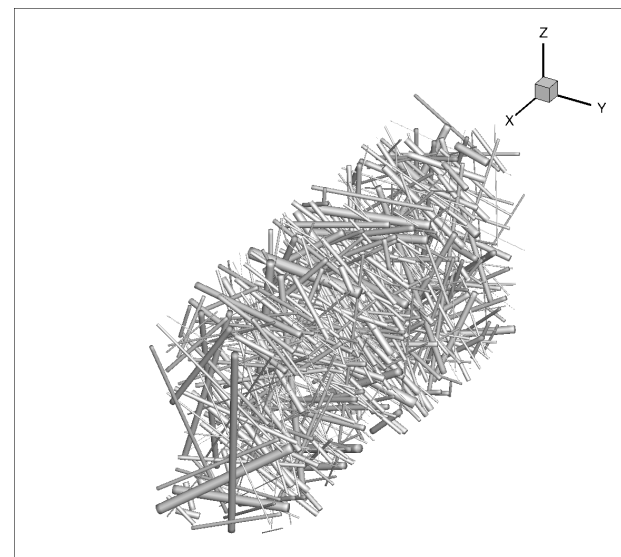
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(a) Non-porous microstructure



(b) Porous microstructure

Figure 1: Fiber-based microstructure created using the FiberGen code [1].

## Qualitative assessment of supersonic flow through porous media with KATS-US

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### Abstract

Modelling the interactions between porous flow and pure flow at atmospheric entry conditions is a challenging task. New models and high fidelity numerical tools are needed to better understand porous material and aerothermal flow interactions for ablation problems. This study presents preliminary results of the development of universal solver (KATS-US) that models both the porous and the pure flow using a single set of governing equations. A set of simulations of a permeable arc-jet test sample is carried out in order to observe the KATS-US capability with proposed model under the supersonic flow conditions. The Arc-Jet test has a porosity  $\epsilon$  0.8 and a permeability  $K$  that varies between  $10^{-2}$  and  $10^{-9}$ . A qualitative assessment of shock formation, porous flow development, pressure change across the porous sample and temperature evolution throughout the porous domain is presented.

**Keywords:** Atmospheric Entry, Porous Flow, Permeability, Darcy's Law, Universal Solver.

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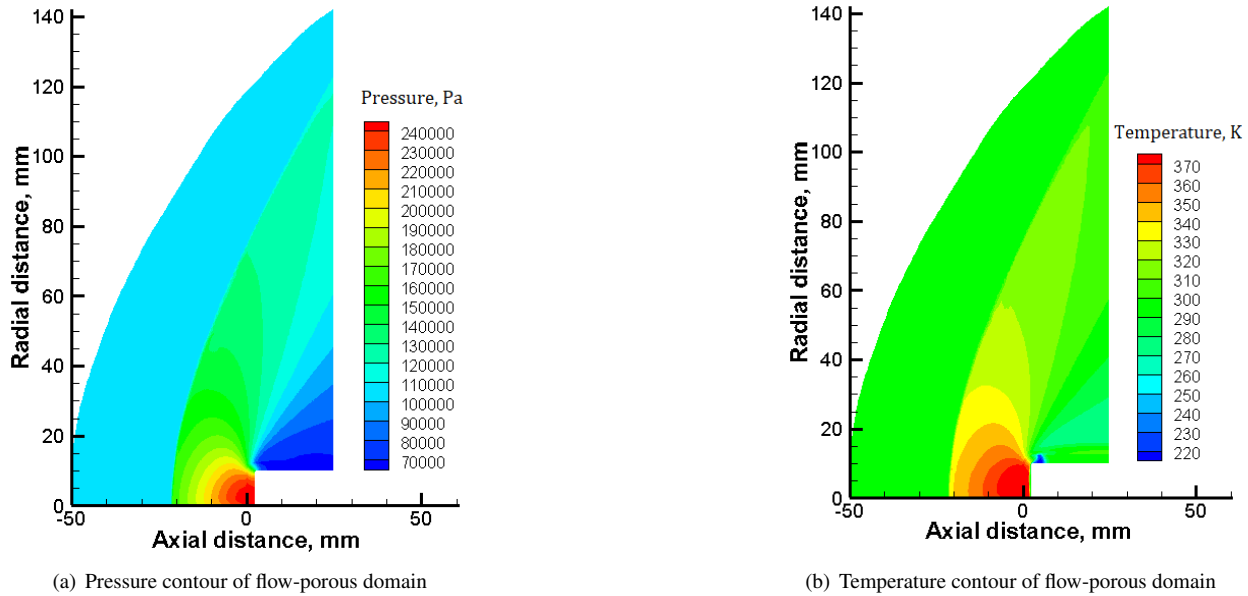


Figure 1: Preliminary results of supersonic flow through permeable material, Mach  $\approx 1.3$ ,  $K = 1 \times 10^{-3}$

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## Modeling multi-phase transport in a porous ablator using KATS Universal Solver

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### Abstract

Historical post-flight analysis from the Apollo program, suggested the occurrence of carbon depositing, or coking, at the outer material layer of the heat shield. In this post-flight analysis, Curry et al. poses an additional solid mass equation dedicated to this mechanism, accounting for the new addition of solid matter via Arrhenius law which only depends on temperature. The present study focuses on this phenomena through the use of the newly developed Kentucky Aerodynamic and Thermal-response System – Universal Solver, or KATS-US for short. KATS-US is a verified finite volume based modeling tool, capable of modeling simultaneously hypersonic flow and material response. To assist in the modeling efforts, KATS-US has been fully coupled with a chemical kinetics solver, Mutation++; thus, capable of carrying out chemical equilibrium calculations on-the-fly at any point within the flow or porous ablator. This study considers a location on a theoretical heat-shield, composed of TACOT, such that a 1-D modeling assumption can be applied, i.e. no measurable effects from the material side walls. Additionally, it is assumed that this sample is impermeable and adiabatic at the back wall, inner-material-layer. The TACOT material database has been refined to incorporate experimentally measured elemental composition pyrolysis data, which has a temperature dependency, for similar materials. As the ablator is pyrolyzed, these elemental potential is equilibrated in its multi-phase state. It is of interest in this study to track this newly generated solid as well as its contribution the materials effective transport properties. A brief qualitative comparison against the Curry et al. data is also provided.

**Keywords:** Heat transfer, Mass transfer, Material response, TACOT

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# Computation of Darcy's permeability in porous media based on voxel images

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## Abstract

Computing to high fidelity the material response of a heatshield during atmospheric entry requires accurate knowledge of its material properties. These are often determined through a combination of experimental and numerical methods. One component of the modeling effort takes place at the micro-scale, based on the microstructural representations of real materials obtained through X-ray microtomography [1]. To analyze these datasets, the Porous Microstructure Analysis (PuMA) software [2] has been developed at the NASA Ames Research Center. PuMA contains modules for calculating effective material properties of porous media, including porosity, specific surface area, thermal and electrical conductivity, and tortuosity as well as simulating oxidation.

This work focuses on the development of a new module for computing permeability of porous media. The steady Stokes' equations are discretized on a staggered grid aligned with the voxels of the 3D tomography image. For porous media with a single phase, cells in the grid are labeled as either solid or void based on greyscale values. The pressure and velocities are assumed to be periodic at the edges of the domain. The method makes use of a standard finite difference stencil with forces applied as corrections at the interface between solid and void voxels. The equations are solved using the biconjugate gradient stabilized method (BiCGSTAB) [3]. The method is demonstrated and verified for a canonical flow around a cylinder, as shown in Figure 1.

**Keywords:** Permeability, Porous Media, Heatshield

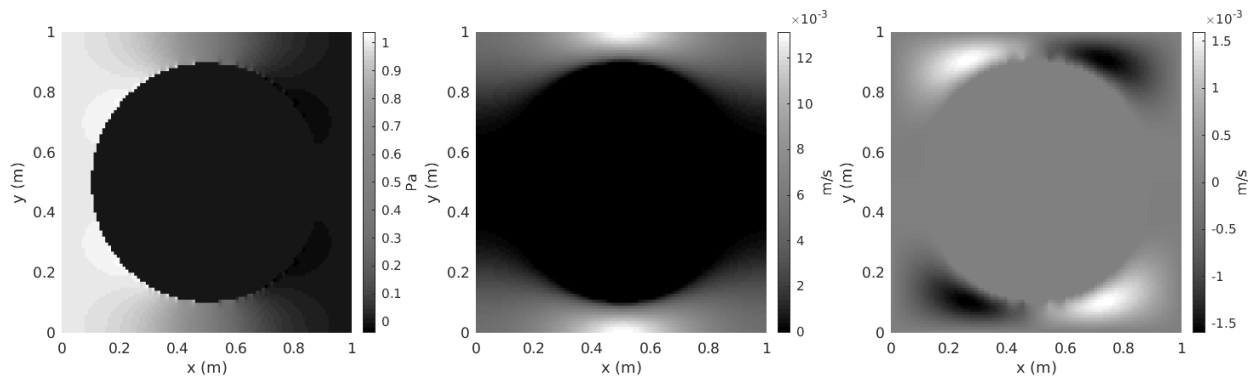


Figure 1: Pressure (left), x velocity (middle), and y velocity (right) fields obtained during permeability computation on a cylinder. The domain size is 100 x 100 cells. The dynamic viscosity and applied pressure difference are set at unity.

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# Conjugate Heat Transfer Model of an Experimental Apparatus Measuring Thermal Conductivity of Fibrous Insulation Materials

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## Abstract

Experimental work has been conducted to measure thermal conductivity of fibrous insulation materials with a comparative cut-bar apparatus. The analysis of these experiments relies on a presumption of one-dimensional conduction through the sample and consequentially negligible radial heat losses from the metering bars. A conjugate heat transfer model of the apparatus has been developed in ANSYS Fluent to verify the validity of this presumption and to provide a means of estimating the experimental uncertainty. This model accounts for radiative, convective, and conductive heat transfer to capture the axial and radial temperature gradients that develop in the metering bar during testing. The expected main sources of heat loss from the metering bar are through the natural convective losses at the sides of the cut-bar and radiative exchange between the cut-bar and enclosure walls. Boundary conditions were set to replicate the experimental conditions by measuring thermocouples placed on the wall of the enclosure and inside the metering bars. Data was gathered for an atmospheric pressure case as well as a low pressure case to determine the effect of natural convection on the experimental uncertainty. The sample material used in the modeling and experiment were made of FiberForm, with the thermal conductivity of the sample material and the thermal contact resistance between the sample and the cut-bars approximated using the preliminary experimental results.

**Keywords:** Heat Transfer, Fibrous, Conductivity, Experimental, Modeling, Fluid, Cylinder

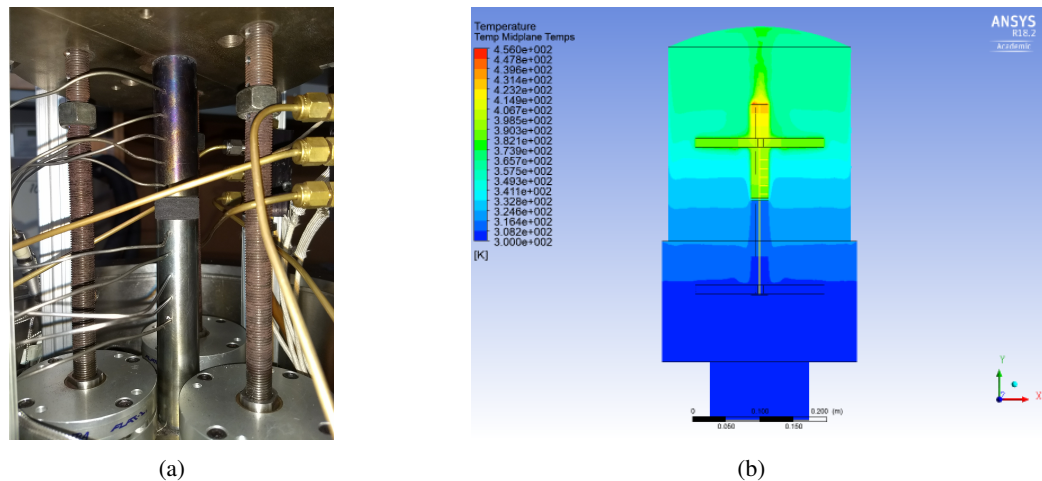


Figure 1: Comparison of (a) experimental apparatus with Fiberform sample and (b) Cross-section of three-dimensional model of experimental apparatus under atmospheric pressure

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## A Thermochemical Model for Oxidation of Ultra High Temperature Ceramics Using High Temperature High Enthalpy and High Temperature Flows

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