11th Ablation Workshop

September 16-17, 2019
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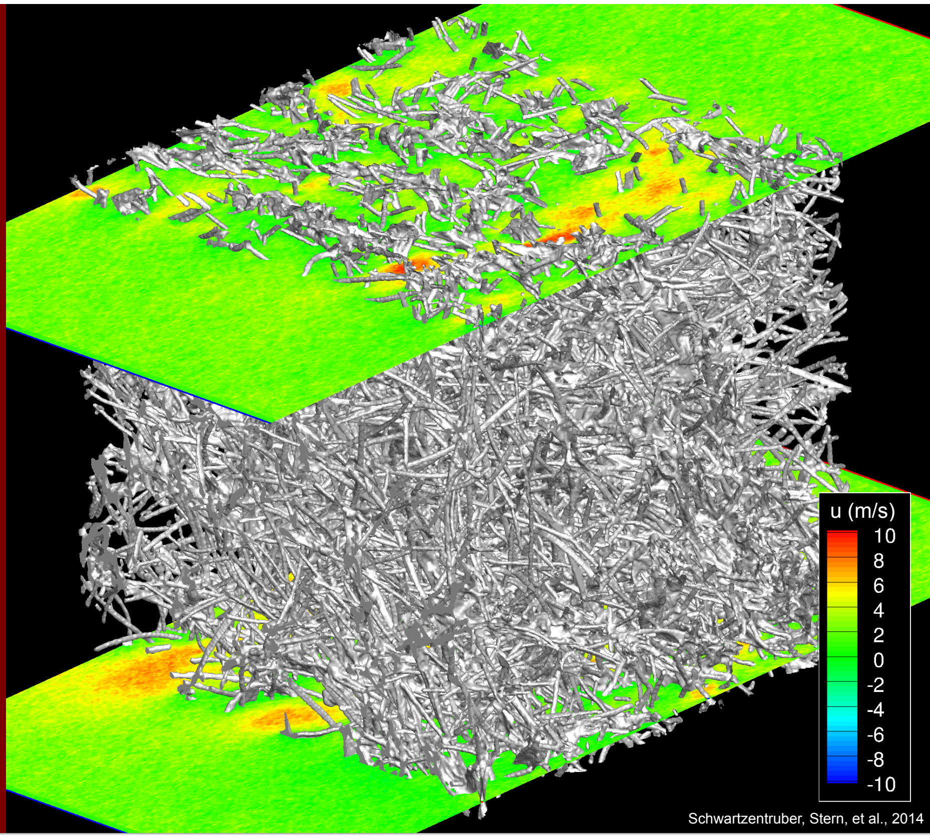

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Overview and welcome

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Overview of NASA ablation activities

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MSR EEV TPS - Requirements, Options, and Trades - What is in, what is out, and challenges ahead

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Recent Developments in Modeling of Ablation Physics at Sandia National Laboratories

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Abstract

Sandia National Laboratories has a long history in the development and application of computational tools designed to solve problems involving ablation and aerothermodynamics. This presentation discusses recent work and future plans that advance the Lab's ablation modeling capabilities.

Since 2013, Sandia has been developing the Sandia Parallel Aerothermodynamics and Reentry Code (SPARC), a computational tool which consists of a fluid solver suitable for hypersonic flows and a material thermal response solver for ablation. We discuss the significant development and V&V the code has seen over the last several years as well as future development efforts. We also introduce next year's effort, which entails a "virtual flight test" of a reentry vehicle – a time resolved reentry trajectory with coupled aero, thermal, and structural response of the entire vehicle.

There are several developments at Sandia meant to improve the predictive capabilities of ablation modeling at the Labs. First, Sandia has revived its ability to manufacture composite thermal protection materials and to characterize those materials in benchtop experimental facilities. We discuss how these efforts are used to improve the predictive capability of decomposing ablators. In conjunction, we discuss mesoscale modeling efforts designed to better understand how to simulate and predict the effective properties of these ablating materials for use in our macro-scale ablation codes, like SPARC.

Approved for unclassified unlimited release as SAND2019-7947 A.

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Material characterization and ablation experiments of the ZURAM® carbon-phenolic ablator for assessment and improvement of selected European material codes

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Abstract

The ongoing technology program on *Ablative TPS Numerical Test Cases Mathematical Code Assessment & Improvement* (AblaNTIS) set up between the European Space Agency, the von Karman Institute for Fluid Dynamics, Samtech s.a. a Siemens Company, and Fluid Gravity Engineering LTD aims at identifying the current capabilities of three selected European material thermal-response codes and to identify their main modelling uncertainties. This will be achieved through the execution of numerical test cases fed by (existing and new) experimental activities performed on the carbon-phenolic ablator ZURAM® [1] including detailed material characterization and plasma wind-tunnel experiments. ZURAM® is recently being developed by DLR Stuttgart for research purposes and presents an ideal candidate for producing experimental data to be internationally shared for ablation test case definition.
After a thorough review of available plasma test data for ZURAM® from previous activities [2], a dedicated test campaign in the VKI inductively-coupled Plasmatron facility has been developed. The new experiments include an updated test sample setup with thermal plug to host in-depth high-temperature (type-B) thermocouples as well as infrared thermography of the surface using a two-color pyrometer, a broadband radiometer and an infrared camera all calibrated up to 3000°C. First experiments have been performed in June 2019 but the test campaign had to be halted in order to overcome an issue with the new setup that we will also present.
Once finalized, the consortium will establish a booklet that will allow anyone external to the project numerical rebuilding of the described test-cases, including suggestions for improved modeling.

Keywords: material characterization, ground-testing and instrumentation, ablation test case definition

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Overview of AFOSR ablation activities

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Microscopic imaging of carbon fiber oxidation in 4D

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Abstract

Predicting oxidation phenomena is critical to the modeling of carbon fiber ablators used in the thermal protection system of hypersonic vehicles. The ablation community is devoting efforts to develop high fidelity computational models for carbon ablation that account for oxidation kinetics at different flight conditions [1,2]. In past investigation we have shown that carbon fibers oxidation can be modeled upon microstructure data of ablators obtained from X-ray computed micro-tomography (micro-CT) [3,4]. The oxidation dynamics in highly porous (>85 %) carbon fiber materials are driven by competing reaction/diffusion processes [3]. At high temperatures, oxidation is in the diffusion-limited regime and ablation occurs as a surface phenomenon. Conversely, at temperatures below 1000 K, oxidation is reaction-limited and material decomposition occurs in depth. In this work, we resolved the oxidation of a rigid carbon fiber preform at microscopic scale using real-time X-ray micro-CT. The material analyzed was FiberForm, a rigid precursor for low density carbon-phenolic materials. We captured the oxidation phenomenon at sub-micron length scale and sub-second time scale, by designing an in-situ high-temperature reactor [5] adapted for the micro-CT setup of the TOMCAT Beamline at the Swiss Light Source (SLS) synchrotron. The reactor was assembled by housing a FibeForm sample in a quartz capillary, surrounded by an outer quartz tube that maintains controlled environmental conditions. The tube was installed to have the sample rotating in the tomography field of view, at the focal point of an array of six gold parabolic-reflector halogen lamps that provide temperatures up to 1200 ºC. High-speed continuous tomographic imaging was achieved with the GigaFRoST X-ray camera system of TOMCAT [6]. This configuration enabled continuous acquisition at several hundred tomograms per experiment. We tested FiberForm samples at temperatures between 900 and 1200 ºC, and pressures from 0.025 Pa to atmospheric, using standard air as test gas. From the high spatial and temporal resolution scans, we could resolve different oxidation processes, from the reaction-limited to the diffusion-limited regime. The data were analyzed using the NASA's Porous Material Analysis (PuMA) software [7].

Keywords: Carbon Fiber, Oxidation, Micro-structure, X-ray Tomography.

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Ablation of carbon fiber TPS samples in DSMC

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Abstract

Historically, many direct simulation Monte Carlo (DSMC) codes, including SPARTA [1], have used triangulated surfaces explicitly defined in an input file to represent the surface of objects in a gas flow. We have developed an alternate surface model where integer values are defined on the corner points of a regular DSMC grid, in similar fashion to the PuMA software [2]. For example, the values can be read from a micro-tomography 3D image file of a complex porous material, such as FiberForm™. A Marching Cubes (MC) algorithm [3] is used with a specified threshold value to implicitly define triangles, each of which is wholly contained in a single grid cell. The figure shows an example of millions of implicit triangles created in this way. We discuss how implicit surfaces were implemented in SPARTA and give performance data for how they can be used in parallel to run models with billions of triangles on thousands of compute nodes. An advantage of the implicit surface representation is that the corner point values can evolve in time, as gas particles collide and react with the surface. The triangulation can then be updated periodically to model recession of the surface. We present preliminary results for a simple ablation model to illustrate how this works, in a similar fashion to Ref. [3]. In the future, more complex surface reaction models, such as oxidation [4] and nitridation models, using intermediate surface species, will be coupled to the implicit ablation model.

Keywords: DSMC, Marching Cubes, Ablation, Massively parallel.

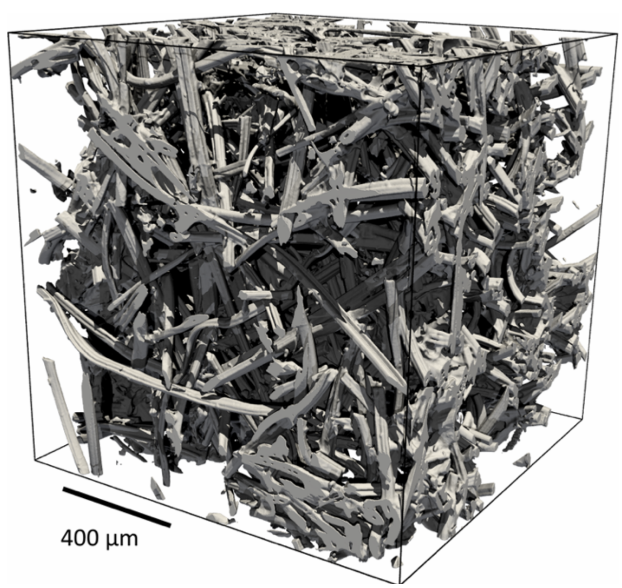

Figure 1: ParaView visualization of triangulated surfaces generated from a micro-tomographic image of a FiberForm™ sample. The original 3D image was from a 0.52 mm^3 cube of material with 0.65 µm voxel edge size; the porosity of the material is 0.856. To create this image, the MC algorithm mapped the voxels to (800)^3 grid cells and produced 57.4 M triangles to represent the surface of the material.

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Image-based mesoscale ablation modeling

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Abstract

The development of next generation materials for thermal protection systems will rely more heavily on simulation than ground testing, in contrast with historical development practices. High-fidelity image-based simulation using as-manufactured materials builds the relation between material mesostructure and ablative performance, fostering rapid development and progress in material design. Addressing the ablation problem at the mesoscale helps characterize the role of material heterogeneities and defects and can inform volume-averaged material response models that are traditionally calibrated to a specific material.

Typically the segmentation of image data is difficult and time consuming. We first summarize our method of image processing and volume reconstruction of a material mesostructure into a finite element mesh with minimal user input and modification. We present an example using a woven composite such that the resulting geometry consists of the fabric weave and matrix phase. Local material orientation is calculated from image texture and embedded in the simulation mesh to capture the anisotropic properties of the composite. Then, using the reconstructed mesostructure, we examine the pyrolysis under an imposed heat flux. Each phase is treated as a porous material where gas and solid phase species are tracked using a mass balance equation allowing for changing density, chemical reactions, dynamic material properties, and pyrolysis gas flow. Pyrolysis is modeled through simple Arrhenius reaction mechanisms in the matrix and weave phase, where an inert fiber background is present in the latter. Temperature evolution is captured through an enthalpy-based porous energy equation accounting for the species present in each phase. Preliminary results of mass loss as a function of material geometry are summarized. Finally, we present initial results on the generation of stresses in the fabric reinforcement throughout the pyrolysis process.

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: Image-based simulation, pyrolysis, mesoscale, woven composites

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Computation of fiber orientation in X-ray Micro-Tomography reconstructions

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Abstract

Due to the fibrous nature of light-weight ablative materials used in spacecraft heatshields, micro-scale modeling has become an important component of the overall material modeling effort. The state-of-the-art simulations to determine the global material properties and response are based on images obtained from X-ray micro-tomography reconstructions. These provide an accurate representation of the material micro-structure. A common assumption in the current models is that the local properties of the constituent phases, such as their conductivity, are isotropic. Although this assumption may be valid for the pore-filling phase, it is not for fibrous and woven structures, often used as the preform for ablative materials. For the computation of the effective thermal conductivity [1], a fully-conservative finite volume scheme based on the Multi-Point Flux Approximation [2] is used, which accounts for the anisotropy of the material at the micro-scale. A requirement of this solver is that the local solid phase orientation is known. This is necessary to correctly align the local property tensor along the fiber orientation. In this study, three methods are investigated: a novel approach based on ray-casting, a method based on the local isotropic heat flux [3] and a common image processing technique called structure tensor [4]. In the ray casting method, rays are created at the center of each solid voxel and travel until the first collision with the interface between solid and void, where the longest path is selected as the dominant direction. The second method imposes a temperature gradient successively in each of the three simulation directions, with a void conductivity of zero and a solid conductivity of unity. The heat conduction equation is then driven to steady state. The normalized local heat flux through these isotropic adiabatic fibers is used as the local fiber direction. The third technique works directly on the grayscale values of the 3D tomography image by computing their gradients at each voxel through the convolution of a Gaussian filter and its derivative. A tensor at each voxel is obtained and the eigenvector, related to the smallest eigenvalue, points in the direction where the grayscales change the least, which is taken as the local fiber orientation. Verification and comparison of these methods' performances are carried out by examining their orientation predictions for artificially generated weaves, whose true local fiber direction is known. These capabilities are implemented in the Porous Micro-structure Analysis (PuMA) [5] software, actively under development at NASA Ames Research Center.

Keywords: woven carbon fiber, fiber orientation, ray casting, thermal flux, structure tensor

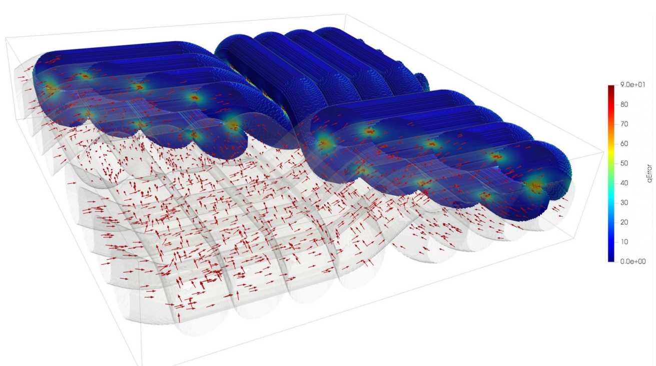

Figure 1: Error between true tangential unit vectors and prediction using the flux method for an artificially generated weave.

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Applying Multiscale Computational Materials Science Methods to Predict Ablation of PICA

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Abstract

In this presentation, we summarize the approach that is being taken at the University of Florida to develop a mechanistic tool to predict the material behavior of the Phenolic Impregnated Carbon Ablator (PICA) material during ablation. In the tool, which is being created using the Multiphysics Object Oriented Simulation Environment (MOOSE), the phase field method is being used to predict the ablation, coupled with mechanics and heat conduction to include the thermomechanical behavior of the model. Material properties needed for the model are being determined using atomistic simulations, including molecular dynamics and density function theory. This approach is summarized in Figure 1. In the presentation, we will provide an overview of our approach and a summary of our current progress.

Keywords: Ablation, Phase Field Method, Molecular Dynamics, MOOSE

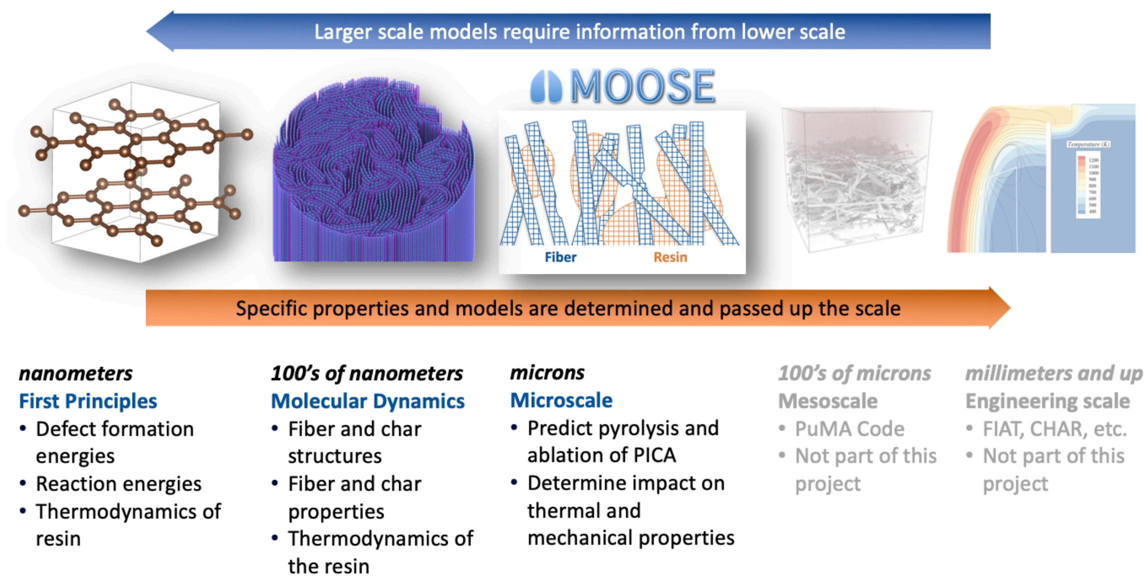

Figure 1: Volume rendering of FiberForm micro-CT (Image taken from Ref. [3]).

Molecular Beam Studies of Carbon and Silicon Carbide Ablation by O and N Atoms

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Abstract

In order to gain a better understanding the gas-surface reactions on heat shields during hypersonic flight through air, we have been using molecular beam-surface scattering experiments to study high-temperature reactions of O and N atoms with model materials. We have conducted extensive investigations of O and N reactions with three types of carbon, (1) highly oriented pyrolytic graphite (HOPG), (2) vitreous carbon, and (3) carbon fiber preform (FiberForm), and work is underway to understand the detailed oxidation mechanisms of silicon carbide (SiC). The experiments were performed with both pulsed and continuous molecular beams of O or N atoms and, in some cases, mixed beams containing O and N atoms.

The reactive scattering dynamics of O on all three carbon surfaces are similar yet the details of the dynamics differ, suggesting that the oxidation mechanisms on all sp^2 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 where the reactions are expected to occur in thermal equilibrium with the surface. In general, we have learned that incoming O atoms increase surface oxygen coverage and lower the barriers to CO and CO_2 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. The reactivity of N atoms on a carbon surface is negligible compared to the reactivity of O atoms until the temperature rises above ~1400 K; then the reactivity of N atoms increases and can become a few percent of the reactivity of O atoms. Even a small percentage of N atoms in the presence of O atoms can increase the reactivity of O atoms on a carbon surface by more than 50%.

the experiments on SiC, we have used 6H single crystal surfaces and have started by preparing oxide layers on these surfaces. Upon heating in vacuum, the oxide layer decomposes 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 an atomic-oxygen beam is directed at the oxidized SiC surface, 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) when the incident O-atom flux is low. But when the O-atom flux is relatively high, the active oxidation regime leads to production of CO and SiO with significant etching of the surface.

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

Visualizing Oxidative and Ablative Erosion of Highly Oriented Pyrolytic Graphite Using Supersonic Beams of O_2 with Scanning Tunneling Microscopy

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Understanding the oxidative and ablative processes in extreme environments that erode carbon-based materials is vital to the design and manufacturing of high-performance aircraft and propulsion systems. To this end, the oxidative erosion and ablation of highly oriented pyrolytic graphite (HOPG) has been visualized with atomic detail using a novel UHV instrument (**Fig. 1**) combining a supersonic molecular beam of O_2 with an *in-situ* scanning tunneling microscope (STM).[1] This unique combination of techniques enables us to tightly control the impinging energy, angle, and flux of the impinging oxygen to elucidate spatiotemporal correlations that govern the evolution of reacting surfaces.[1,2] It was observed that different oxidation conditions lead to morphologically and kinetically distinct etching properties of the surface: anisotropic channels, circular pits, and hexagonal pits faceted along crystallographic directions (**Fig. 2**) all form at different surface temperatures and impinging energies and angles of O_2. The probability of an impinging O_2 molecule removing a carbon atom from the HOPG surface demonstrated non-Arrhenius behavior with respect to surface temperature, peaking around 1375 K. Reactivity significantly increased with an increase from 0.4 to 0.7 eV in the translational energy normal to the surface of the impinging O_2 molecules; the angle of impingement demonstrated only minor effects on the reactivity of the surface. The evolution of etch channels on the surface was kinetically dominant at all studied surface temperatures and represents a mechanism activated at higher impinging O_2 energies, presumably due to an increased concentration of adsorbed oxygen on the surface.[3] Comparison of the morphological evolution and relative reactivities of higher grade versus lower grade HOPG surfaces indicates that the formation of etch channels is due to the presence of intrinsic grain boundaries. Multilayer etch features were visualized and the vertical etch rate was found to increase significantly with an increase in surface temperature, which has been experimentally observed previously under different oxidative conditions.[4] Structural defects and surface inhomogeneities were found to play an integral part in the reactivity and morphological evolution of the reacting surface. For example, the insertion of

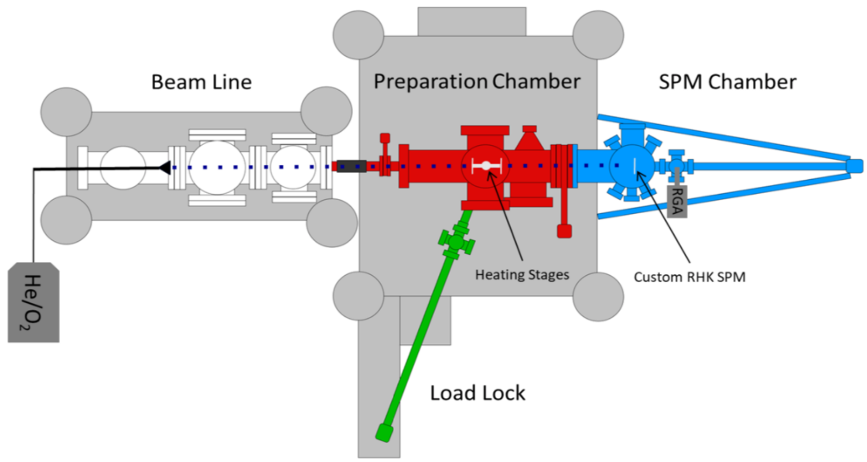

Figure 1. A schematic of the custom UHV instrument containing both a supersonic molecular beam and *in situ* scanning tunneling microscope.

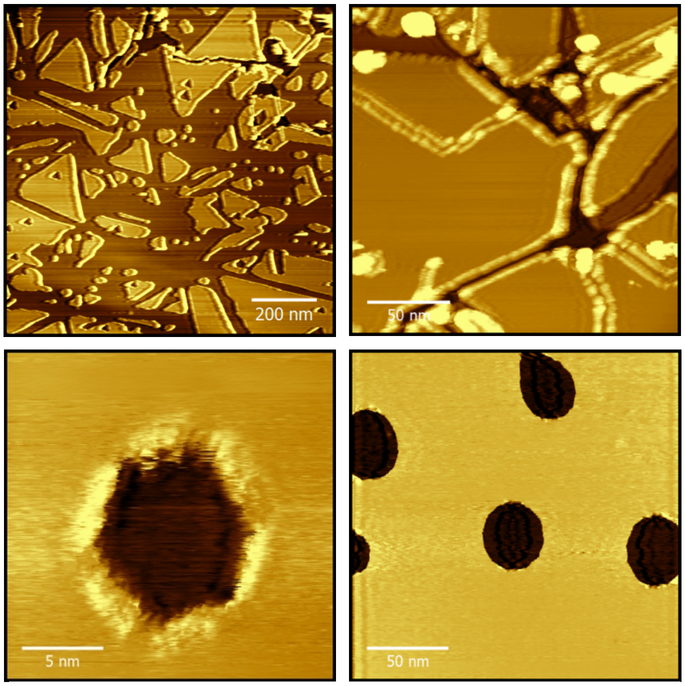

Figure 2. Representative STM images of different morphological features formed on the HOPG surface after exposure to 0.7 eV O_2 at 1275 K (top left) and 1375 K (top right), and 0.4 eV O_2 at 1275 K (bottom left) and 1375 K (bottom right).

intentionally created point defects via ion sputtering leads to marked enhancement in interfacial reactivity. The nucleation time for reactivity decreases significantly with the introduction of these point defects, and computational studies have demonstrated the importance and role of these defects on the dissociative chemisorption of the impinging O_2 molecules.[5] The approach presented in this talk has allowed us to correlate the time-evolving morphological evolution of the surface with atomic-level interfacial reaction dynamics, providing new insight into the reactivity of carbon-based materials in aggressive, energetic environments.

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Finite rate modeling of reactions between dissociated air and carbon at high temperature

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Title:

Kinetics Model of Graphite Ablation Rates as a Function of Microstrostructure

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Abstract:

Graphitic materials are of interest for applications such as thermal protection systems of hypersonic vehicles owning to their high oxidation and ablation resistance in extreme environments. While there is a vast amount of information from literature on their oxidation and ablation behaviors, very few analyses address the effect of microstructure (in terms of surface chemistry and defect density) on reaction kinetics for different types of graphite and carbon-based materials. In the present work, we investigate the ablation behaviors of highly ordered pyrolytic graphite (HOPG), isotropic graphite (I-85), and 2D woven carbon-carbon composites (C-C) in an high temperature isothermal oxidizing environment using a thermogravimetric analyzer (TGA) at both the reaction rate limited and diffusion limited kinetic regimes. While the three materials have similar mass loss rates within the diffusion controlled regime at 1600 °C, they exhibit very different ablation rates within the reaction rate limited regime at 650 °C, with HOPG hardly experienced any mass loss during the oxidation test period. In order to gain more insight on the entire ablation process including gas flow over the sample and the potential oxidation reactions occur at the sample surface, it is necessary to correlate the diffusion of various gaseous species to the oxidation reaction kinetics. By combining the empirical results including mass loss rates measured by DNE-TGA, microstructural characterizations using a scanning electron microscopy (SEM), and surface chemistry and defect structures, diffusion behaviors of oxygen (O_2) and gaseous products (i.e. CO and CO_2) across the gas boundary layer are simulated through computational fluid dynamics (CFD) modeling and incorporated for kinetics modeling using Thermo-Calc DICTRA software. Partial pressures of various gas species at the carbon/gas interface are estimated from the experimental data as well as material microstructures (i.e. surface chemistry and defect structure) and are used as inputs for the models. By doing so, we are able to engage the microstructural effect with the mass loss rate (which is dictated by the diffusivities of the gases) for the three different graphitic materials, and meanwhile, predict their ablation rates at various conditions.

An Interface for Coupling Icarus to the US3D Flow Solver

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Abstract

Material response-flow coupling is a critical capability for accurate simulation of hypersonic vehicles and atmospheric entry systems. Examples of NASA projects which have need for such a capability include the Mars Sample Return (MSR) mission where MMOD strikes during return to Earth pose a risk to TPS reliability, and Asteroid Threat Assessment where massive ablation greatly influence the aerothermal environment. In addition, if an efficient implementation of flow coupling can be developed, it circumvents the need for the contrived boundary layer assumptions that go into typical decoupled TPS simulations, while enabling the deployment of higher fidelity finite rate surface chemistry models. While there have been several successful effort to *demonstrate* coupling, the resultant software has yet to be infused in the design process. To this end, the development of an interface for coupling the Icarus material response solver [1] to the US3D hypersonic CFD code [2] is presented. With the release of US3D v1.1, the solver now supports the development of plug-in software modules. US3D plug-ins provide a convenient and flexible way to extend the capabilities of US3D, and, in contrast to the previous user subroutine paradigm, multiple plug-ins can be used simultaneously. This talk will describe the on-going development of a US3D plug-in to enable coupling of the Icarus ablative material response code. The current state of the plug-in will be demonstrated through a relevant benchmark geometry and trajectory, and on-going and future developments discussed.

Keywords: Ablation, Computational Fluid Dynamics, Atmospheric Entry

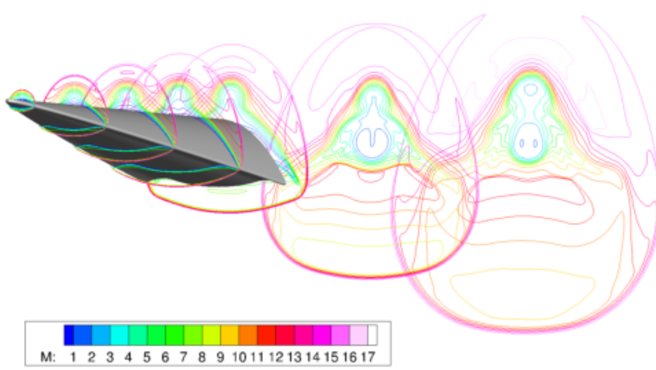

Figure 1: Visualization of the Waverider geometry used to demonstrate coupling capability.

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Unravelling the mysteries of porous transport properties

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Abstract

Keywords: Bourbon, thermal response, toasting, charring, chemical decomposition

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Additive Manufacturing of Ultra-Performance Polymers for Thermal Protection Systems*

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I. Introduction

There has been an increasing interest in developing polymeric materials that are compatible with additive manufacturing (AM) processes and that could be used as a thermal protection material for spacecraft. The goal of this research is to develop a novel class of materials and additive manufacturing processes that could substantially reduce the manufacturing and assembly costs of spacecraft thermal protection systems (TPS) as heat shield. As AM increasingly gains commercial and academic interest, government agencies, such as NASA seeks to produce TPS using Fused Filament Fabrication (FFF) method. In this study, a total of five materials using three different ultra-performance polymers, including polyetherimide (PEI), polyetheretherketone (PEEK), and polyetherketoneketone (PEKK) were tested and evaluated for thermal, flammability, and ablation properties while maintaining compatibility with commercially available FFF machines. The four neat ultra-performance polymers used were SABIC ULTEM™ 9085, Roboze PEEK, Smartmaterials3D PEEK, and Arkema Kepstan® 7002 PEKK, and a modified PEI (ULTEM™ 1010) material [1]. These five polymers were characterized with thermogravimetric analysis (TGA) for thermal stability and char yield, and microscale combustion calorimeter (MCC) to determine flammability properties. After obtaining and analyzing TGA and MCC results, test specimens were then fabricated using 1.75 mm diameter FFF filaments with commercially available high-temperature 3D printers. Ablation test models (dome-shaped 20 mm diameter cylinders and dome-shaped 30 mm diameter cylinders) were printed via FFF using oxy-acetylene test bed (OTB) for aerothermal ablation testing. These FFF ablation test models were then evaluated for ablation and thermal properties using the OTB at low heat flux test conditions simulating reentry conditions, such as 100 W/cm^2 for 15s, 30s, 60s, and 120s. From these aerothermal ablation tests, the materials' recession, mass remainder, surface temperature, and backside heat-soaked temperature were recorded. Furthermore, microstructural analysis was performed using scanning electron microscopy (SEM) to study the microstructures of printed test specimens. In order to fully exploit the experimental data provided by the OTB, the flow field generated during aerothermal testing using this heat source was recently modelled by the Koo Research Group. CFD analysis using Ansys/Fluent 19.1 code to analyze the heat transfer between the ablative surface and the combustion gases generated by the OTB and compared with experimental results.

II. Experimental Approach

The five materials were evaluated using TGA for thermal stability and char yield properties. MCC instrument was used to study the five materials' flammability properties. These five materials were then fabricated into FFF ablation test models and evaluated for ablation and thermal properties using the OTB. Test models of 30 mm diameter dome-shaped and in length were tested at realistic test conditions simulating reentry conditions, such as 100 W/cm^2 for 15s, 30s, 60s, and 120s. From these aerothermal tests, the materials recession, mass remainder, surface temperature, backside heat-soaked temperature, high-definition and IR surface temperature videos were recorded.

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To prevent severe side heating which causes problems for ablation testing of 3D printed FFF test models [2], a modified OTB setup was established. An extension tube made of stainless steel was used to hold the sample (Figure 1). This also reduced the risk of overheating the metal chuck holding the samples. A type K thermocouple inside the tube was inserted to the backside of each sample to measure heat-soaked temperature.

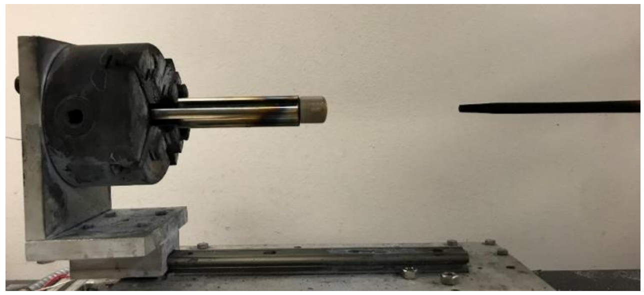

Figure 1. Modified OTB setup for ultra-performance polymer AM parts.

A. Thermal Stability and Char Yield Property Results

A graphical representation of degradation temperatures at 10% mass loss and 30% mass loss are shown in Figure 2. The ULTEM™ PEI polymers reach 10% and 30% mass loss at lower temperatures than the PEEK and PEKK materials, which indicates that the thermal stability of PEI is lower in comparison to PEEK or PEKK. Arkema PEKK lost 30% of its mass at the highest temperature of 640℃. The degradation curves of the ultra-performance polymers are shown in Figure 3. ULTEM™ 9085 begins to degrade first among the polymers, whereas Roboze PEEK and Smartmaterials3D PEEK begin to degrade last. It is observed that Arkema PEKK degrades before the PEEK materials but begins to stabilize before the PEEK materials at around 630℃. This degradation curve highlights that ULTEM™ 9085 is the worst performer, while Arkema PEKK has the best results.

B. Flammability Property Results

MCC tests were performed on the candidate materials and a summary of the MCC results is shown in Figure 4. The HR capacity, peak HRR, and peak temperature as well as the corresponding standard deviations (SD) are recorded in parenthesis next to value. Based on the MCC data, SABIC ULTEM™ 9085 and Arkema PEKK appear to be the superior materials in terms of flammability properties. Though SABIC ULTEM™ 9085 shows better heat release (HR) compared to PEKK, these two materials can be deemed to be similar in flammability performance due to a larger SD on the data of SABIC ULTEM™ 9085. However, PEKK stands as the best material among others because of its lowest heat release parameters and highest peak temperature, which can lead to best stability under extreme temperatures. Comparing the two ULTEMs, SABIC ULTEM™ 9085 slightly outperforms Modified SABIC ULTEM™ 1010 in flammability properties as evidenced from HR Capacity. In addition, SABIC ULTEM™ 1010 shows slightly higher peak temperature. Moreover, in the comparison of those two PEEKs in this study, Roboze PEEK shows better flammability property than Smartmaterials3D PEEK while they yield equal peak temperatures. Overall, the MCC results conclude that PEKK is the best material in terms of flammability followed by ULTEM™ 9085, and modified ULTEM™1010, respectively.

C. Aerothermal Test Results

It is observed that all five specimens experienced various amount of swelling/expansion during the OTB testing. For all materials tested, HD camera video footage shows that the pyrolysis zone has been established at the center of the specimen after the first 5s of exposure. As exposure time increases, the charred surface keeps accumulating and slowly expands further. It is noted that none of the charred samples fell apart even after 30s exposure, all samples kept its structural integrity. After 30s exposure, the two PEEK materials show the lowest level of expansion whereas the modified ULTEM™ 1010 have the highest value change in thickness. Both ULTEM™ materials exhibit low peak heat-soaked temperature for both 15s and 30s tests, which could be correlated to their char formation and morphology. Both post test samples of ULTEM™ exhibit a highly porous char surface. Taken into account the fact that the two PEEKs also have the highest peak heat-soaked temperature, it is possible that the volatile decomposition products during pyrolysis can cool down the surface temperature by acting as a heat sink to. Future studies are needed to support this observation. Figure 5 shows the post-tested OTB test models after all the lose chars were removed by a wire brush.

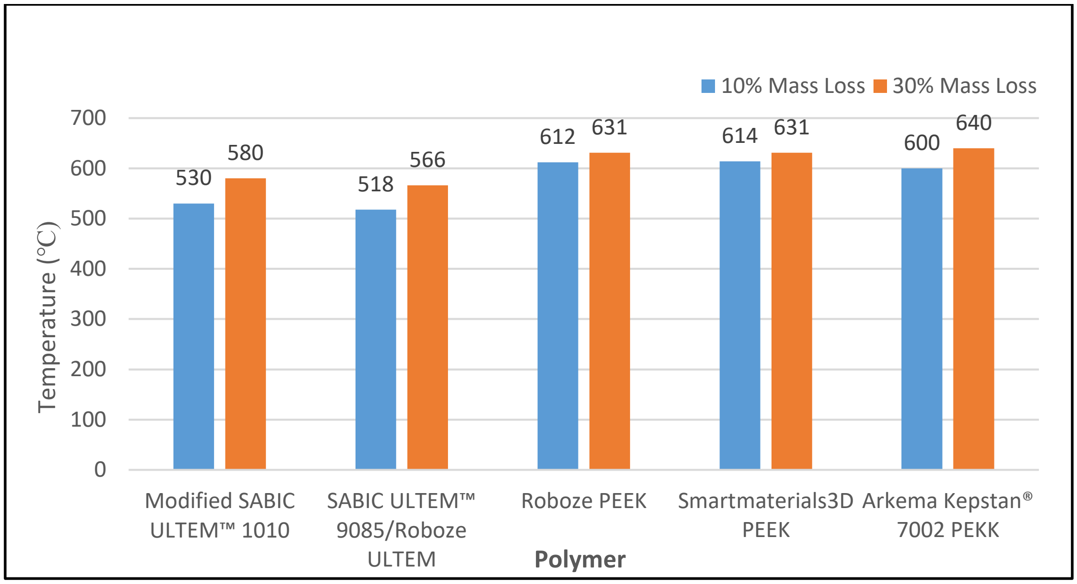

Figure 2. Graph of decomposition temperatures at 10% and 30% mass loss.

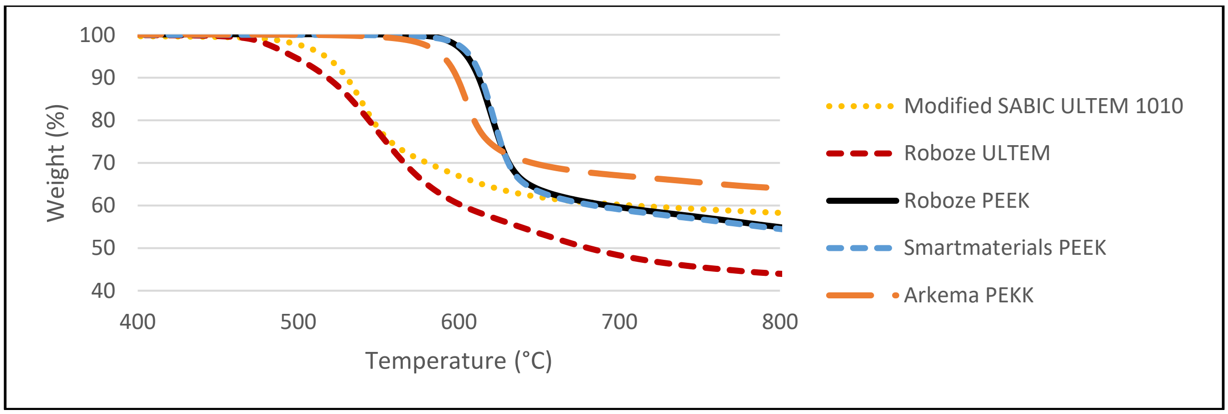

Figure 3. Graph of degradation curves of ultra-performance polymers (TGA, heating rate of 20°C/min in N_2).

Figure 6 shows that all five materials loss their mass in a linear fashion as exposure time increases. At 30s, PEKK has the highest mass residue left whereas the ULTEM9085 has the lowest. As time reaches 120s the discrepancies between different materials become more obvious. Overall, all five ultra-performance thermoplastic materials were able to withstand OTB testing at a heat flux of 100W/cm^2 for as long as 120s without disintegration. The specimen geometry plays a role in the sample decomposition during OTB combustion. The mass loss for the 15s tests are similar for all five materials and char morphology could be correlated with the exposure time. For 60s tests, the extra 15s doubles the mass loss percentage for all five specimens among which PEKK shows the lowest mass loss. A higher peak heat-soaked temperature and lower peak heat-soaked time is also observed but it does not significantly affect the char thickness and surface temperature during combustion. More tests are in progress in order to better understand the ablative performance and thermal properties of the selected materials.

III. Numerical Studies

In order to determine the fluid flow and heat transfer between the combustion gases and the candidate material, modified ULTEM, a numerical analysis was performed by using the Ansys/Fluent 19.1 code [3]. In this study, a steady-state analysis was performed to determine the fluid flow using the turbulence model of k-omega SST, because fluctuating velocity fields can be small scale and high frequency, and direct simulations of these fluctuations can be very expensive in terms of computational calculations. The numerical study was converged by second order implicit scheme and pressure-based solver. The mass flux convergence criteria for steady-state solution is approximately 10^{-5} level. Non-premixed combustion model was used in order to simulate the combustion of acetylene and oxygen. For the first step, a geometry which illustrates the physics of the problem is constructed.

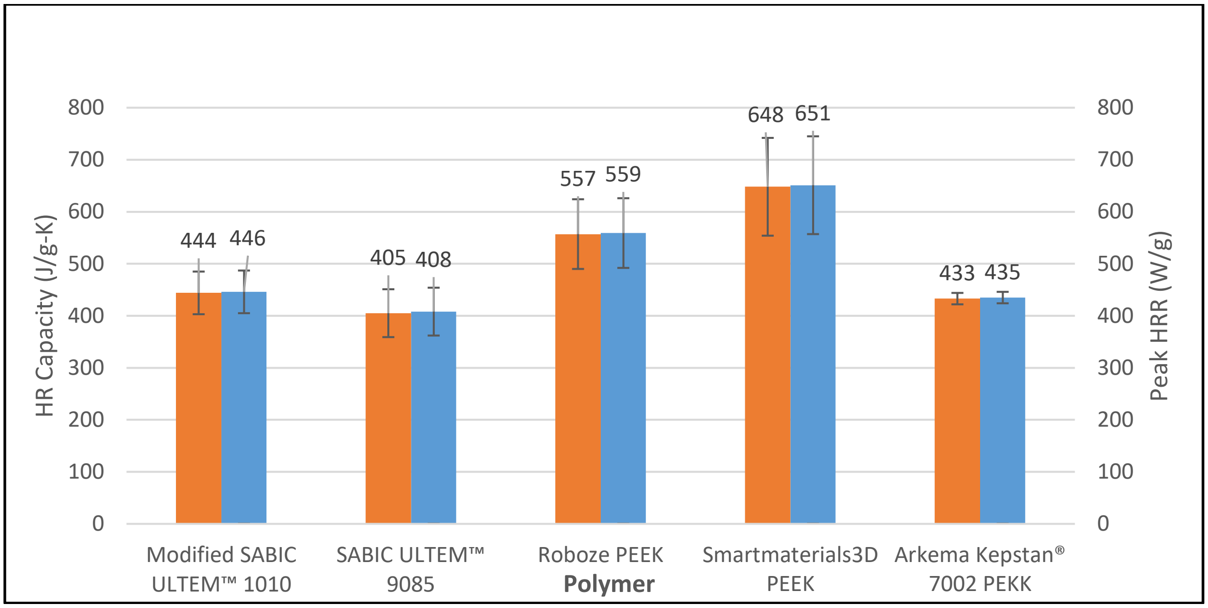

Figure 4. Summary of MCC HR capacity and peak HRR results.

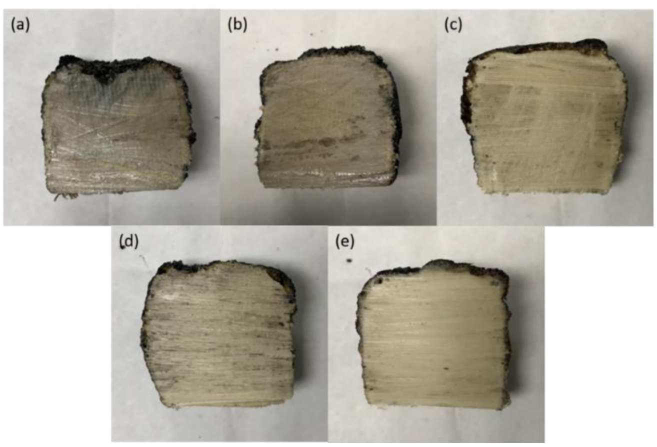

Figure 5. Cross section of AM printed parts after 30s of OTB testing: (a) PEEK Smartmaterials3D, (b) PEEK Roboze, (c) PEI ULTEM™ 9085, (d) PEI Modified ULTEM™ 1010, and (e) PEKK.

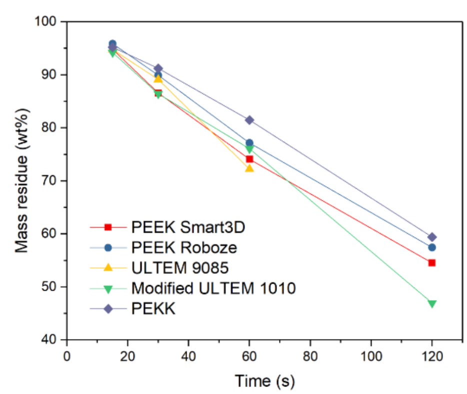

Figure 6. Mass residue vs. time plot for five FFF printed polymers for different test durations.

Mass flow rate of the fuel is given as a boundary condition and acetylene and oxygen are mixed in the torch. Oxygen and acetylene ratios of the mixture are determined from the experimental conditions. Velocity and temperature profiles of the OTB setup are calculated. According to results, maximum velocity value appears at the exit of the nozzle part. Output gases hit the surface of the ablative material and are reflected from the surface to the sides. For 100 mm standoff distance; the maximum velocity of the gas is approximately 2,100 m/s, the maximum velocity of the combustion gas hitting the front face of the ablative material is ~ 319 m/s, and a maximum temperature of is ~ 2,595K. This is a result of steady-state simulation of flowfield. For the heat flux determination, an unsteady analysis was performed. This study presents a simulation of heat transfer in an oxy-acetylene test setup. Heat flux between the ablative material and combustion gases is calculated by an unsteady analysis. According to experimental test, approximately 105 W/cm^2 heat flux was measured at a standoff distance of 100 mm. The results between the experimental data and numerical simulation compare well.

IV. Concluding Remarks

Results from the 120s OTB tests will be provided for a more complete understanding of the ablation performances of the five materials. Simulation results for all five materials will also be compared and discussed. The team will conduct close-up photo and Scanning Electron Microscopy (SEM) analyses on the post-test materials to observe their microstructures for better understanding of the mechanisms of their ablation performances and working computer models for their simulation.

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Multi-scale Thermal Response Modeling of an AVCOAT-like Thermal Protection Material

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Abstract

A multi-scale modeling approach based on the stochastic Direct Simulation Monte Carlo (DSMC) and random-walk methods is developed [1] to understand the complex flows and thermophysical phenomena through a syntactic foam TPS, similar to AVCOAT, which is shown in Fig. 1(a). At the kinetic level, collisions between boundary layer and pyrolysis gases with each other as well as the internal material microstructure directly affect the material thermal response through changes in the thermal and the bulk velocity components of the gases, thereby affecting the convective heat fluxes imposed not only on the spacecraft surface but also on the interior portions of the microstructure. These, in turn, potentially affect the conductive and radiative fluxes carried through the material. Also, when the contribution of gas transport to the material thermal response is considered at the micro-scale level, the internal, local Knudsen number varies from transitional to continuum due to the small material length scale even when the external hypersonic flow around the spacecraft is entirely continuum in nature. Therefore, one objective of this work is to stochastically obtain the convective fluxes by taking into account the interaction of boundary layer and pyrolysis in DSMC. The second objective is to address the critical question regarding the relationship between the TPS material's microstructure and its thermal response. In syntactic foams subjected to high temperatures, the conductive and radiative heat transfer is strongly coupled and understanding of this coupling can provide insights that can potentially benefit the ablation community. Therefore, we use a stochastic, random walk approach that builds upon a method proposed by Vignoles [2, 3] to study coupled conduction and radiative heat transfer mechanisms in porous materials with complex morphologies. We present an extension of this approach to the case where the material thermophysical properties of thermal heat conductivity, heat capacity, and density have large variations, consistent with the characteristics encountered for heat shield materials and demonstrate the required computational parameters for a one-dimensional heat transport model.

To simulate counter flows of boundary layer and pyrolysis species through a complex three-dimensional morphology, a hybrid CPU-GPU DSMC solver, CHAOS [4], based on unstructured, adaptively-refined, octree grids is discussed. The use of the DSMC approach with the proposed material model is demonstrated in terms of its ability to directly calculate the permeability and tortuosity through AVCOAT for two different porosities. To relate the DSMC inlet and outlet species boundary conditions to those of larger length scales provided by material response solvers and to accurately model the low velocity flows inside the material, a general approach for high temperature, subsonic boundaries is discussed. Figure 1(b) shows the three-dimensional domain setup for DSMC, where the left and right-hand side boundaries are inlet and outlet, respectively. Note that the boundary layer species enter from the left side (z) and the pyrolysis species enter from the right side (-z) of the domain.

Furthermore, our implementation of the walker approach through a syntactic foam is described in Figs. 1(b) and 1(c). The material is discretized into 'plates' which are analogous to 'cells' in a finite volume formulation, along the direction of the depth in which the temperature gradient is significant. Initially, N_w^{tot} number of walkers are distributed among all the plates based on the initial fractional enthalpy of those plates. Then, a stochastic differential equation [5] corresponding to the Fokker-Plank equation of the normalized probability density of walkers [6] is solved numerically using the Euler-Maruyama approximation [7]. A comparison of the random-walk approach with one-dimensional, finite-volume MR solutions is provided when both conduction and radiation are included and the required number of walkers, N_w^{tot}, to obtain statistically converged solutions for this class of heat transfer problems is also established. Finally, using these approaches, the contribution of conductive heat transfer is compared with con-

vection, and the effect of including the DSMC derived convective heat fluxes in the walker thermal response method is compared with the finite-volume approach.

Keywords: Thermal protection system, Ablation, Porous media, Material thermal response, DSMC, Random walk, Pyrolysis, Conduction, Radiation, Permeability, Gas-surface interactions, Gas-gas collisions

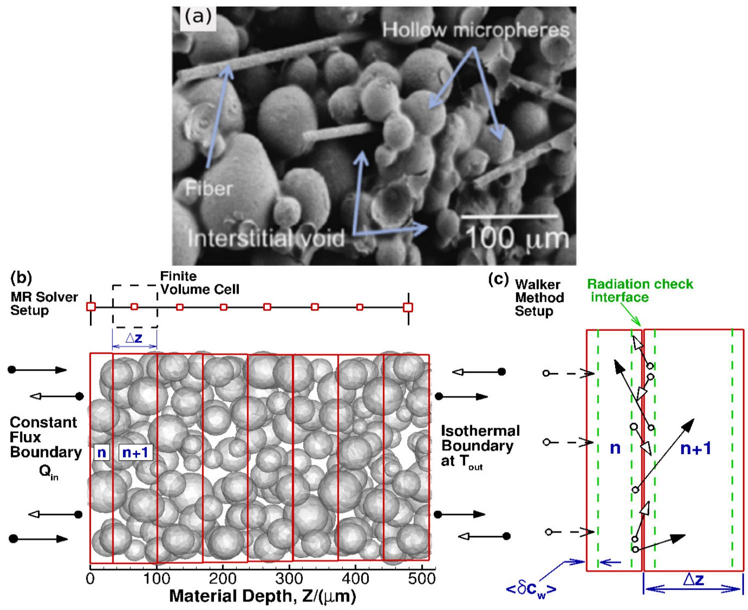

Figure 1: (a) Scanning electron microscope (SEM) image of AVCOAT sample [8], (b) A computer aided design (CAD) of microstructure approximating the SEM image with the one dimensional plates used in the walker simulations and finite volume cells for the MR solver. The DSMC simulation computational particles (filled circles) are designated by solid and hollow headed arrows for the boundary layer and pyrolysis species, respectively. (c) Schematic of the walker model showing walkers (unfilled circles) that are introduced to simulate a convective heat flux boundary (dashed arrows) and the evaluation of walker representation as radiative or conductive heat carriers (solid vs. open arrow heads) performed at the interface between two plates. [1]

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Phenolic polymer pyrolysis via reactive molecular dynamics simulation

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Abstract

Pyrolysis of phenolic polymers is studied with reactive MD, using various ReaxFF parametrizations in order to improve the accuracy of modelling of phenolics in extreme environments. Bauschlicher, et al., 2013 has demonstrated that the commonly used Chenoweth CHO parametrization could be improved with better quantitative agreement with DFT of barriers and reactions energies of common pyrolysis byproduct reactions. That evaluation was based on ReaxFF energies of DFT-optimized structures. In this work, the energies associated with these mechanisms are re-evaluated with reactive path analysis, based on ReaxFF-determined structures. The results are compared across three ReaxFF parametrizations: two previously published and a newly developed, hybrid parametrization that we show accurately models phenolics in the mechanical compression regime. Additionally, constant temperature, constant volume MD is carried out at various temperatures between 2000 and 3250 K to elucidate reaction rates of two processes that occur during phenolic pyrolysis–the liberation of volatiles and the production of water–to enable an Arrhenius analysis and a comparison with experimental data.

Keywords: phenolic polymers, molecular dynamics, ReaxFF.

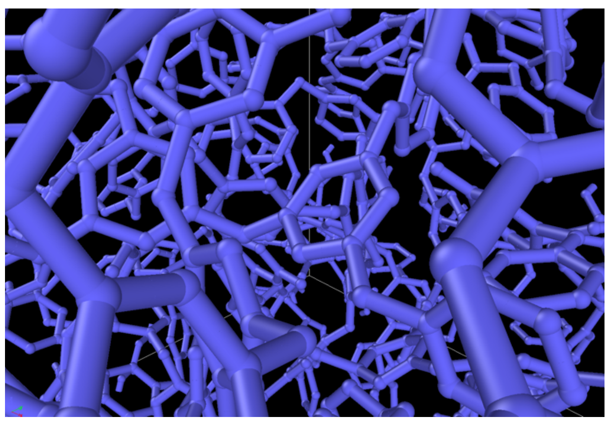

Figure 1: Molecular dynamics snapshot of a crosslinked phenolic polymer.

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A coupled DSMC-SPH solver to study atmospheric entry ablation in presence of a rarefied gas phase

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Abstract

Debris from launcher stages and satellites at end-of-life is increasingly becoming a threat for humans when remains, that have not fully disintegrated during descent, impact the ground. The development of prediction tools for space debris demise and risk assessment requires a description of the entrainment of the molten layer into the hypersonic rarefied flow, where the different fluid phases cannot be described by the same models. On the contrary, the solid and liquid can be treated as continuous media, whereas a kinetic treatment is needed for the gas.

In our approach, both phases are simulated by particle schemes: the Direct Simulation Monte Carlo (DSMC) [1] for the gas phase and the Smoothed Particle Hydrodynamics (SPH) [2] for the solid and liquid phases. While DSMC is the dominant technique for rarefied gas flows simulations, SPH has been selected, among other numerical techniques, because of its mesh-free Lagrangian nature which allows dealing with free surfaces naturally. Thermal and dynamic coupling between the gas and the condensed phase is obtained by applying classical kinetic boundary conditions for the vapour, at the interface. Momentum and energy are exchanged between liquid and gas after the interaction of the molecules of gas with the free surface.

In this work, we present the details of the coupling methodology, along with some verification test cases, e.g. a slab of material melting under the effect of a supersonic Couette flow, for which a semi-analytical solution can be found in slip regime. Finally, we consider the melting of a solid cylinder immersed in a hypersonic stream. The dynamics of the formed molten layer under the influence of the rarefied flow is analysed.

Keywords: Melting, space debris, multiphase flow

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TPS technology maturation and sustainment in support of in-situ science missions: HEET and PICA

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Review of Airborne Observation and X-ray Analysis of the Hayabusa SRC Heatshield and Future Plan for the Hayabusa2

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Abstract

Asteroid Explorer Hayabusa2 has successfully carried out touch-down on the Asteroid Ryugu and will return to the earth with asteroid samples in the end of 2020. After successive trajectory correction maneuvre being carried out, the SRC (sample return capsule) separated from the spacecraft enters the earth atmosphere with the velocity of about 12 km/s. Passing through the severe aerodynamic heating corridor, SRC will jettison both of the forebody and aftbody heatshields and deploy the parachute at the altitude of about 10km. Airborne fireball observation is planned during the reentry flight both for acquiring emission spectroscopic data of the heatshield and for reconstruction of the reentry trajectory [1]. In order to make maximum use of the current rare opportunity of the super-orbital reentry, the outcome of the former Hayabusa SRC is briefly overviewed: The fireball observation concluded that recession due to sublimation was trivial if existed based on the observed surface temperature. According to the recession measurement by the 3D laser scanning system of the recovered heatshield, severe recession was not measured while the expansion is measured in some portion of the surface[2]. JAXA spectroscopic measurement for the Hayabusa2 SRC are under being designed especially in the bandwidth of the 4-color filter system [3] in order to improve the accuracy of estimation of the surface temperature of the heatshield during the reentry.

Keywords: Hayabusa SRC, Heatshield, Ablator, Airborne Observation, X-ray tomography

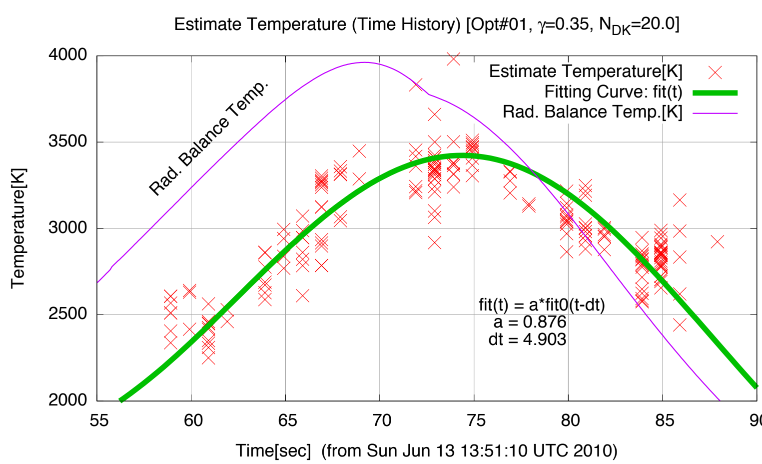

Figure 1: Surface Temperature Estimation of Hayabusa SRC during the reentry (Image taken from Ref. [4]).

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An Analysis of the Hypervelocity Impact Response of Graphite and an Overview of Weather Capabilities at the NASA WSTF-RHTL Facility

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Abstract

The facilities at the Remote Hypervelocity Test Laboratory at NASA White Sands Test Facility provide an opportunity to test the impact response of relevant hypersonic materials to projectiles moving at extreme speeds. The test parameters may be tuned to simulate exo-atmospheric impacts or potential weather encounters during flight. The facility can operate over a range of temperatures spanning -196°C to 2000°C while maintaining an instrumentation suite that characterizes the projectile velocity, the specimen temperature, and the evolution of the impact event. As a demonstration of both high-temperature operation and a three-dimensional particle tracking algorithm, a set of fine-grain graphite specimens were shot with a field of aluminum spheres moving at 4.50 km/s. The evolution of the impact event and the trajectory of each particle relative to the sample surface were observed and measured using calibrated high-speed cameras. Specimen temperatures were measured using both a type-C thermocouple and pyrometry. Surface morphology and crater diagnostics were performed post-test with a white-light interferometer.

Keywords: Particle Impact, Orbital Debris, Graphite Erosion, Computer Vision

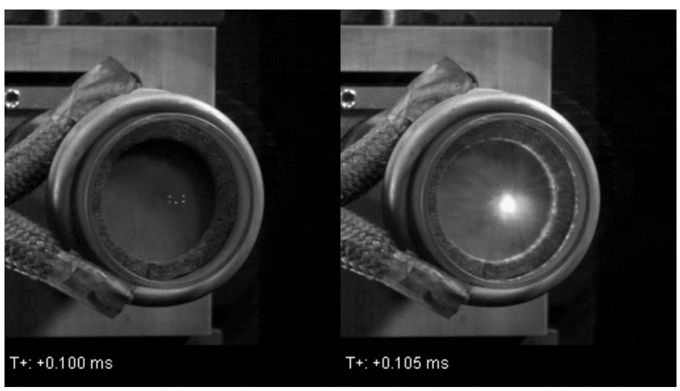

Figure 1: Image of the graphite sample immediately prior to and during impact

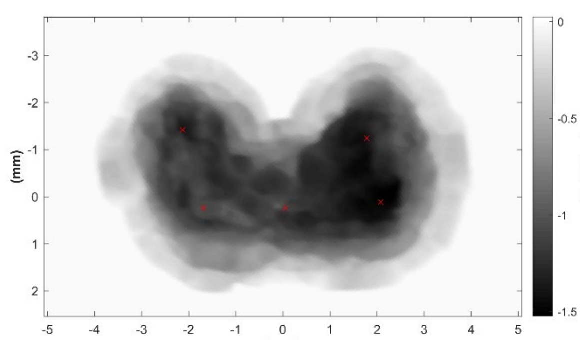

Figure 2: Depth map of the post-test surface taken on a white-light interferometer

Ablation Chemistry Under High-Heat/High-Flux Solar Testing

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Abstract

Phenolic impregnated carbon composites are ablative thermal protection system (TPS) materials that have a rich history in the development of ablation mechanisms [1,2]. To aid in TPS materials development and gain further insight to ablation mechanisms (e.g., pyrolysis chemistry; char depth, etc.), a series of phenolic based samples were prepared and tested for a joint experimental and computational modeling program. Samples were made from carbon fibers and the phenolic based resole resin (SC-1008). Characterization of both the constituent materials and composite were provided for mesoscale modeling efforts. Both laboratory bench top analysis and high temperature/high flux heating at Sandia's National Solar Testing Facility were used to support thermophysical characterization. Materials testing under extreme environments using a new solar furnace chamber (propriety design) was performed to collect and evaluate pyrolysis products garnered under controlled atmospheres. Using this new tool, results are being evaluated against proffered ablation mechanisms.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Keywords: Thermal Protection System (TPS), Carbon Phenolic (CP), Ablation, Pyrolysis,

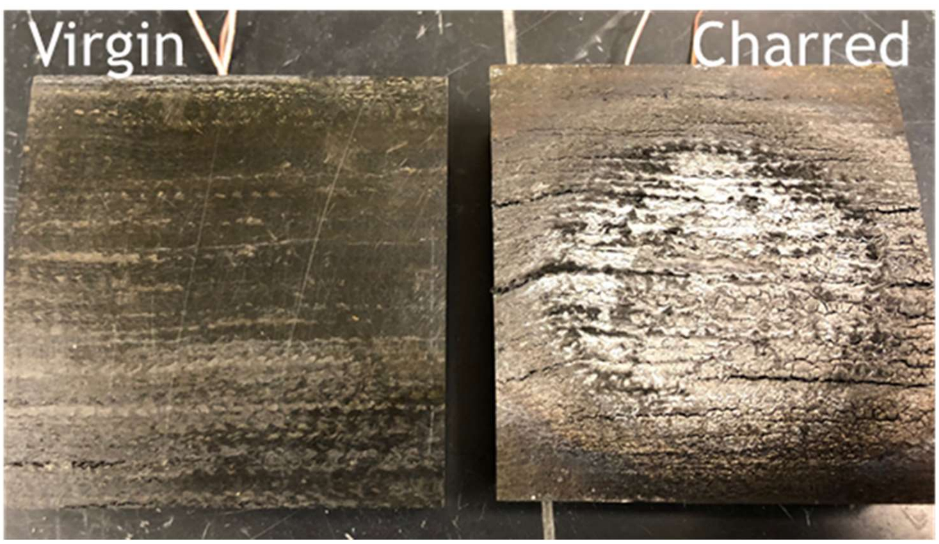

Figure 1: Comparison between a Virgin and Solar Furnace Charred Sample

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An Ultrasonic method for ablation rate measurement of Silica-Phenolic TPS material

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Abstract

Re-entry and hypersonic vehicles, as well as rocket engines, are exposed to extreme heat loads, shear forces, and chemically aggressive gases. To protect the vehicle, ablative thermal protection materials are commonly used. These materials ablate and lose mass, and as a result change in thickness and shape. That directly affects the insulating and aerodynamic performance of the vehicle. Hence, during testing and certification of thermal protection materials, its critical to monitor and evaluate their ablation performance.

In this study, a non-destructive ultrasonic measurement method is proposed for monitoring the ablation process and measuring the residual thickness of Silica-Phenolic TPS material. Generally, in ultrasonic methods the pulse transit time is measured, and based on a known speed of sound the material thickness can be evaluated. In composite materials, as in Silica-Phenolic, ultrasonic pulses are refracted, scattered and reflected from the material inhomogeneities. Moreover, during the ablation process, heat conduction within the material causes a change in its structural properties and consecutively a change in the speed of sound. Several studies in the past have dealt with this problem either by evaluating the temperature varying speed of sound inside the material [1] or by using a phased array transducer to simultaneously correct for speed of sound change during the test [2].

The method presented in this study uses and extends the work of Lloyd et al. [3]. Their approach was based on monitoring the diffuse ultrasound backscatter from the internal micro-structure of Carbon-Phenolic and some woven TPS materials. Monitoring and tracking in time-domain the shift of the backscattered echoes can be used to directly compensate for influence of temperature and material properties change on the speed of sound without modeling. In addition, when the temperature dependency of the speed of sound is known, this method provides a way to estimate the temperature distribution within the material during the ablation event.

We will present the results obtained with the method described above using Silica-Phenolic TPS material tested in a Oxy-Acetylene torch apparatus. In addition, we will show a way to verify the backscatter tracking method by embedding artificial reflectors within the material. Tracking the echoes from the reflectors provides a way not only to verify the ablation and temperature monitoring, but potentially to use it in materials where the backscatter is not significant. For illustration, raw ultrasonic scans of ablation of two Silica-Phenolic samples are presented in Figure 1. The upper image is a scan of the base sample and the bottom is the scan of a sample with three reflectors embedded at different depths.

Keywords: Ablation, TPS materials, Ultrasound, Backscatter

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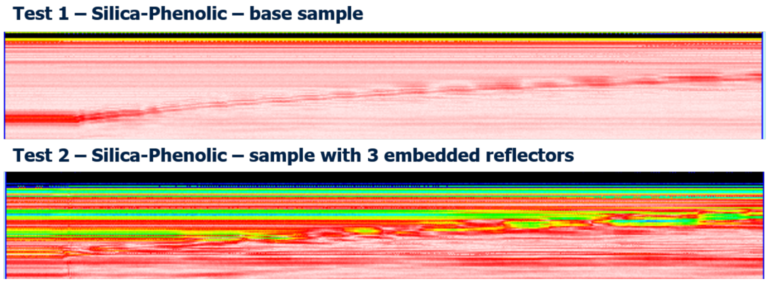

Figure 1: Ultrasonic scan of Silica-Phenolic sample ablation

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Analysis of the PICA-NuSil HyMETS Arc-Jet Campaign

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Abstract

Thermal Protection Systems (TPSs), such as Phenolic Impregnated Carbon Ablator (PICA), receive a thin coating of silicone resin to control particle shedding before assembly in clean room environments. A commercially available siloxane coating (NuSil CV-1144-0) was applied to the surface of the Mars Science Laboratory (MSL) heatshield and the integrated sensor plugs of the Mars Science Laboratory, Entry, Descent, and Landing Instrument (MEDLI). Post-flight analysis of MEDLI data has not considered the presence of the siloxane coating as its effect on TPS performance is expected to be negligible. However, pre-MSL arc-jet qualification testing of MEDLI coupons revealed a surface temperature discontinuity, a feature that is not considered with state-of-the-art materials response models.

An experimental test campaign has been carried out at the Hypersonic Materials Environment Test System (HyMETS) arc-jet facility, at the NASA Langley Research Center, to inform the development of high-fidelity materials response models. Mini-sprite models, coated with different thicknesses of siloxane coating, were subjected to several test atmospheres (e.g., Air, Nitrogen, and CO_2), and various heat flux conditions. Temperature measurements of siloxane-coated mini-Sprite samples show a surface temperature discontinuity when tested in air and nitrogen environments.

A four-stage mechanism is proposed to explain the observed surface temperature discontinuity (fig. 1). In stage 1 (blue box), the surface temperature instantaneously rises to 1600 °C, and the siloxane resin pyrolyzes to form a thin silicon oxycarbide (black glass) coating. In stage 2 (green box), the temperature stagnates at 1600 °C, a protective layer of SiO_2 forms as the surface oxidizes. Additionally, the underlying silicon oxycarbide layer separates into domains of SiC, SiO_2, and graphite. In stage 3 (red box), the temperature rises as carbothermic reduction reactions initiate the breakdown of the stable surface coating, exposing the underlying char to the boundary layer and subsequent exothermic carbon-oxidation reactions. As the surface temperature reaches a steady-state (stage 4, yellow box), the carbon char ablates at a faster rate than the relatively stable silicon oxycarbide layer to yield uneven recession at the surface of the TPS.

Keywords: Ablation Chemistry, PICA, Silicon Oxycarbide, Carbothermic Reduction.

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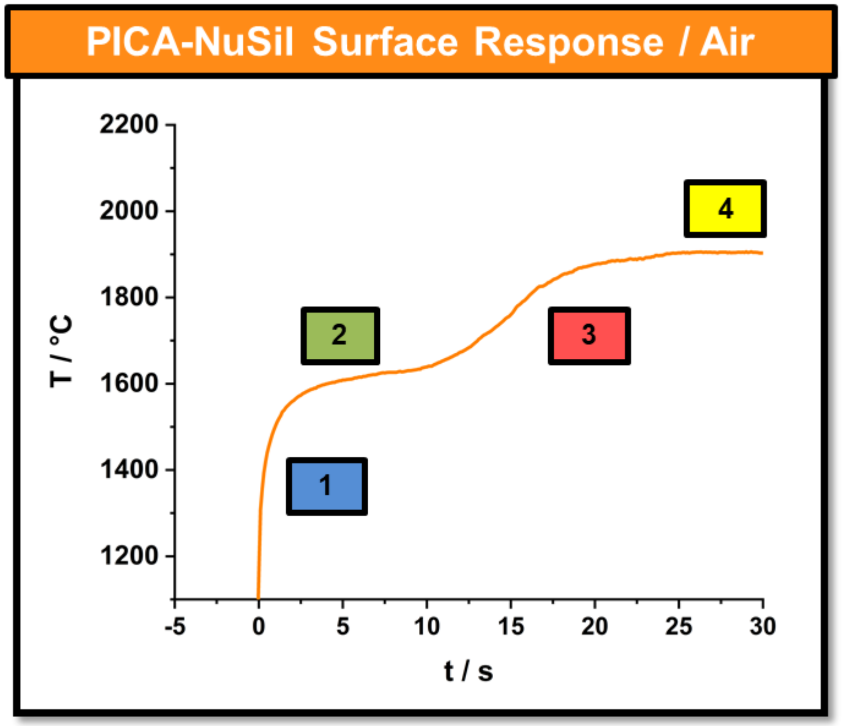

Figure 1. The surface temperature profile of a mini-sprite model during arc-jet testing. The profile clearly shows a temperature discontinuity that begins at ~ 1650 °C.

Recombination of Nitrogen Atoms on High-Temperature Graphite

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Abstract

To verify the high carbon nitridation rate by measured by Park and Bogdanoff in their shock tube experiment [**?**] SRI International and the University of Vermont (UVM) collaborated on experiments in two different test facilities. The SRI group used a diffusion sidearm reactor facility that measured the gradient of atomic nitrogen produced by a microwave discharge as it diffused toward high purity graphite using two-photon laser-induced fluorescence at pressures of 1-5 torr and graphite temperatures of 873 to 1373 K. From these tests, the reported nitridation efficiency ranged from $0.2(10)^{-3}$ at 873 K to $9.8(10)^{-3}$ at 1373 K [**?**] . At the same time, similar measurements of relative N atom mole fractions in an inductively coupled plasma (ICP) torch facility at UVM showed evidence of a high rate of N atom depletion near the graphite surface, as shown below in Fig. 1. From absolute number density and the carbon mass loss measurements from the test, the nitridation efficiency was found to be $6.45(10)^{-3}$, albeit at a higher surface temperature of nearly 1500 K, in reasonable agreement with the results of SRI. However, the N atom depletion could not be explained by this low nitridation rate. From an analysis of the relative mole fraction and temperature gradients [**?**], the overall nitrogen atom depletion rate was determined to be 59.8 ± 14.9 m/s. After accounting for the nitridation rate of 2.51± 0.44 m/s, the remaining depletion rate of 57.2 ± 14.9 m/s was attributed to nitrogen atom recombination. Evidence of nitrogen recombination was found by comparing absolute emission from N_2 (1+) vibrational features at 1 mm and 2 mm above graphite and quartz in the nitrogen plasma.

Keywords: Nitrogen recombination, carbon nitridation, nitrogen plasma

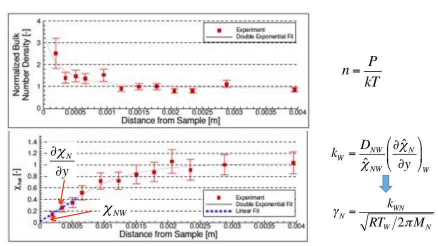

Figure 1: Nitrogen atom distribution above graphite surface. (Image taken from Ref. [**?**]).

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Investigation of Thermochemical Processes in Inductively Coupled Plasma Torches

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Abstract

Inductively coupled plasma (ICP) facilities are increasingly being used to validate new gas-material chemical kinetic models for heat shield materials. Characterizing the state of the plasma inside the torch and determining the thermodynamic conditions will provide key inputs to hypersonic CFD solvers to enable validation of the new models. To meet this objective, simulations have been performed using the *nonPDPSIM* platform, a 2-dimensional, non-equilibrium plasma hydrodynamics model [1]. The plasma transport module (charged particle continuity equations and Poisson's equation), the electromagnetic module (2D frequency domain solution for coil generated electric fields), and the fluid module (Navier Stokes equations) were combined in a time-splicing manner until the steady state is reached. The plasma torch at the University of Vermont is simulated, where spectroscopic data is being collected for validation purposes. A schematic of the torch and number densities are shown in Fig. 1, which demonstrates the formation of a localized plasma near the coils. A region of strong non-equilibrium occurs near the coils, where the electron and excited state number densities are significantly higher than nominal equilibrium values. However, the number densities decrease rapidly in the radial direction because of plasma symmetry-the azimuthal electric field on the axis is zero. The localization of the plasma quantities also localizes the power deposition inside the coils resulting in gas temperatures greater than 10,000 K in a very narrow region around the coils, and the hot gases are then convected downstream by the fluid motion inside the coils [2].
Keywords: NonEquilibrium plasma physics, Characterizing freestream conditions in ICP.

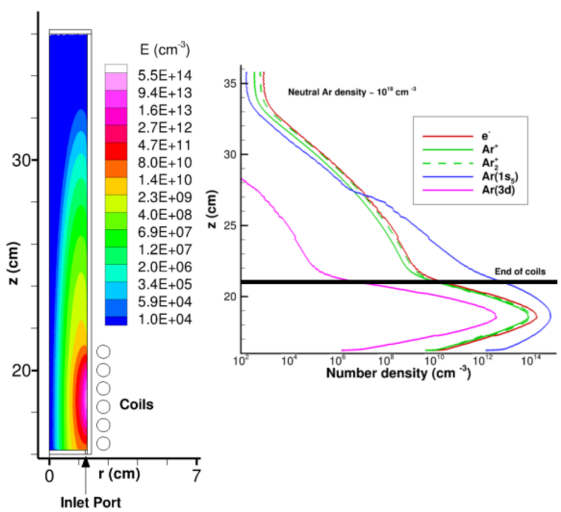

Figure *1*: Schematic of the plasma torch with the number density of electrons (left) and the number density of electrons and excited states at r = 1.75 cm (right).

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Oxidation of Silicon Carbide in coupled, reacting boundary layers

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Abstract

Ultra-High Temperature Ceramic (UHTC) materials, including silicon carbide (SiC), are of interest in hypersonic vehicles due to their refractory nature and high thermal conductivity. However, oxidation continues to be the limiting factor, contributing to material degradation and loss of re-usability. This work summarizes the progress on modeling SiC oxidation in air environments, with applications to computational fluid dyanamics (CFD) and material response simulations.

A gas-surface model for SiC oxidation based on thermodynamic equilibrium has been developed and validated [1]. Passive-to-active oxidation transition conditions predicted with this approach are compared to experimental data in oxygen and air [2, 3] in Fig. 1(a). When coupled to material response analyses of SiC-coated composites, the temperature jump phenomenon observed in ground test experiments [4] is predicted within 8% of pre and post-jump temperatures. Within a coupled non-equilibrium CFD framework, detailed boundary layer chemical kinetics and the effect on surface properties are also investigated in hypersonic flight conditions, particularly the surface energy balance illustrated in Fig. 1(b). Figure 1(c) compares the simulated emission spectra from the oxidizing boundary layer (computed using NEQAIR [5]) to the data of Panerai et al [4].

Ultimately, this work lays the foundation for future experimental comparisons and further investigation of the non-equilibrium gas-surface processes.

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

References

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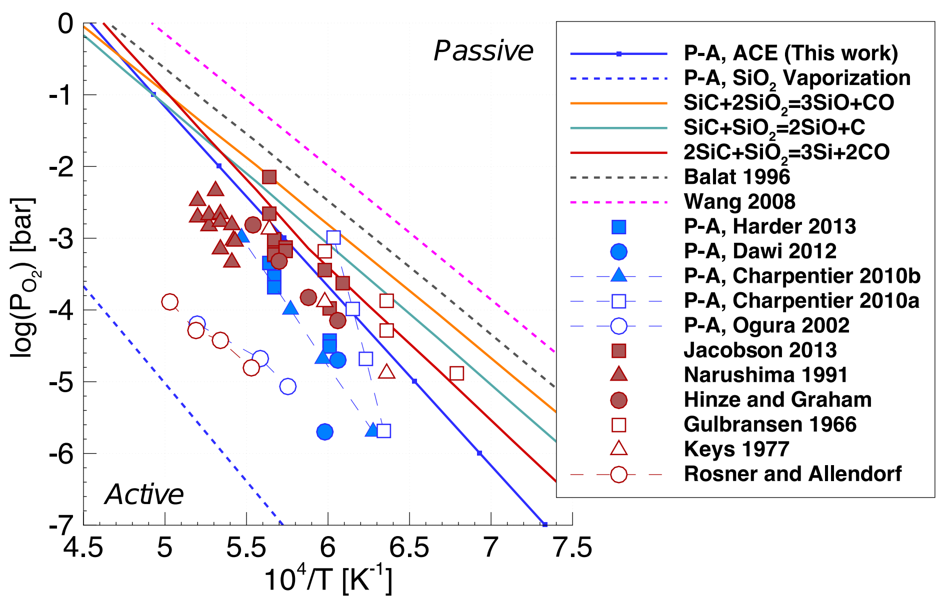
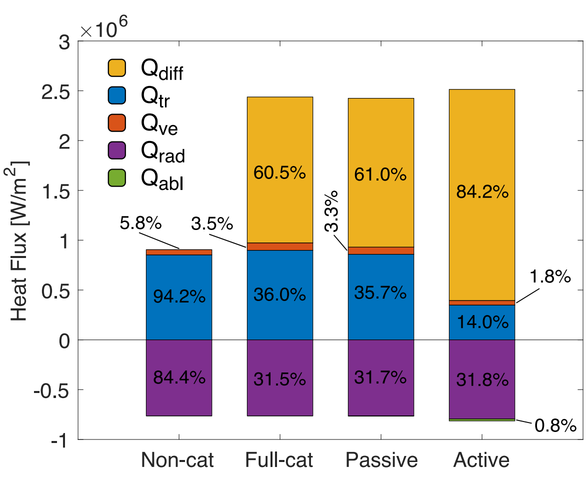
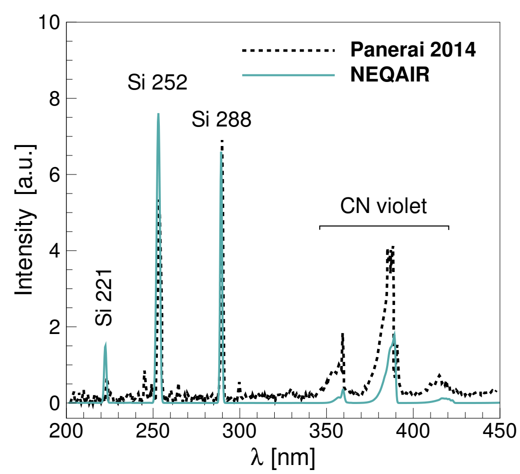


(a) Arrhenius plot of passive-to-active transition conditions



(b) Stagnation point surface energy balance at 25 MJ/kg



(c) Boundary layer emission spectra from CFD and NEQAIR

Figure 1: Silicon carbide oxidation model and results.

Catalytic recombination in the Mars atmosphere

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Department of Mechanical Engineering - University of Vermont

As part of the Mars Pathfinder Program, Mitcheltree [1] developed a surface catalysis model for Mars entry applications, which consists of the following parallel reactions:

$$\begin{aligned} O + (s) \rightarrow O_s \quad &\Longrightarrow \quad CO + O_s \rightarrow CO_2 \\ CO + (s) \rightarrow CO_s \quad &\Longrightarrow \quad O + CO_s \rightarrow CO_2 \end{aligned} \qquad \text{(a)}$$

This model ignores the possible competing recombination to form molecular oxygen:

$$O + O \rightarrow O_2 \qquad \text{(b)}$$

Sepka, et al. [2] investigated surface reactions (a) and (b) on quartz (a low-catalytic material) in a side-arm reactor. Their measurements clearly indicated that reaction (b) occurred much more readily than reaction (a), which implies that further oxidation of CO to CO_2 by the surface is unlikely. This finding also suggests that the Mitcheltree model and, consequently, the super-catalytic assumption are overly conservative. However, numerical simulations of heat flux measurements from wind tunnel tests suggest that the super-catalytic recombination model is correct [3]. Such contradictory results justify the conservative TPS design assumption of super-catalycity and warrant further investigation. The talk will present the latest details on efforts at UVM to look for evidence of CO_2 formation through Diode Laser Absorption Spectroscopy (DLAS) at the surface. We have already developed the DLAS system [4] and have improved its sensitivity with better photodetectors and support equipment. Materials known to have catalytic and non-catalytic behavior for CO_2 recombination will be used to elucidate the relative efficiencies of proposed recombination paths. A cold wall platinum surface will serve as a reference catalytic material. Additional tests will be performed using quartz and copper samples providing data for less catalytic surfaces. Tests of all materials will include TALIF measurements of CO and O atom concentrations near the surface to resolve their fluxes and recombination efficiencies (as in [5]).

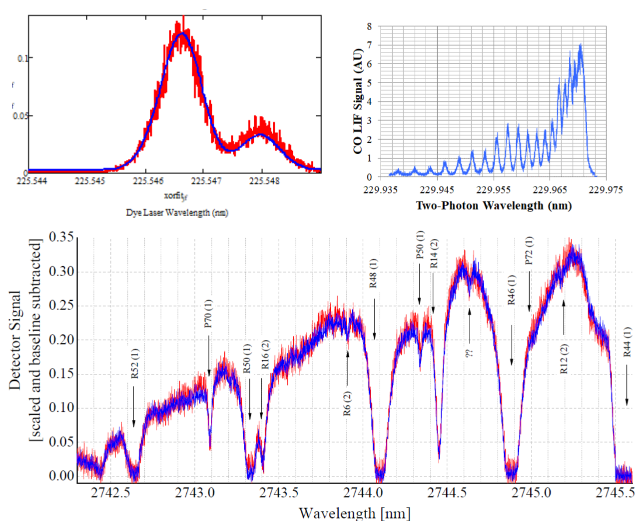

Figure 1: Top Left: O atom TALIF using SFM. Top Right: CO ro-vibrational TALIF using SFM. Bottom: DLAS trace of CO_2.

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Validation of carbon ablation models based on Plasmatron experiments

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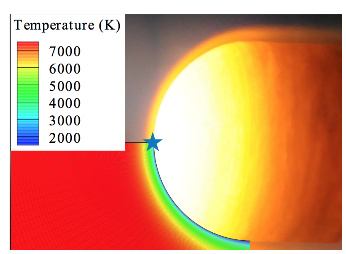
Abstract

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++ library [1]. Both ablative and catalytic processes are considered for a broad range of fidelity levels, from detailed chemistry reactions at the material surface to local thermodynamic equilibrium conditions. Abstracting GSI phenomena in a library can make them easily accessible to researchers for straightforward code-to-code comparison. MUTATION++' 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.

The developed GSI module was coupled to in-house CFD solvers to study carbon ablators based on experiments performed in the VKI Plasmatron facility. A spherical sample of a fiberform (CBCF by Mersen) was placed in the high enthalpy jet for several conditions, allowing us to assess its ablative properties (Ref. [2]). The experimental results were numerically reproduced taking into account the surface phenomena of oxidation, nitridation and sublimation. One of the main aims of the simulations was to compare a state-of-the-art detailed surface chemistry model for carbon oxidation [3] with the more commonly used phenomenological models [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. The influence of nitridation was particularly assessed based on tests of pure graphite in a nitrogen plasma. A model for nitridation was developed, while the coupled effects of thermal nonequilibrium and ablation was also studied.

Keywords: Oxidation, Nitridation, Surface balances, Mutation++

(a) CBCF preform sample.



(b) Simulation of the plasma flow around sample.

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Micro-tomography and Modeling Based Reconstruction of the High Temperature Behavior of Meteoritic Material in Air: Implications for Entry

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Abstract

Meteoroids are made of a complex assortment of minerals that lead to a heterogeneous heating and ablation during atmospheric entry. Here, the behavior of chondrites, stony meteoroids that are amongst the most common to enter the atmosphere, are investigated at high temperature through synchrotron X-ray micro-tomography, computational materials techniques, and material response simulations. In-situ high-temperature experiments were performed by heating chondrite samples to 1200 K in a tube furnace installed at the micro-tomography beamline of the Advanced Light Source at Lawrence Berkeley National Laboratory [1]. Tomographic reconstructions of the material at increasing temperature were used to examine the internal structure of the material and quantify the evolution of Ni- and Fe-rich grains, troilite compounds, micro-cracks, and porosities. Unexpectedly, regions of material were found to vaporize, leaving traces of solid material in surrounding cracks as shown in Figure 1. A computational analysis of the melting point and reactivity with oxygen for the primary mineral components of chondrites suggest that the missing regions are FeS (troilite). The melting point of troilite is larger than the experimentally examined temperature, but the reaction of troilite with oxygen is highly exothermic and can lead to the evolution of gaseous sulfur dioxide and molten iron. The behavior of this reaction mode during atmospheric entry was evaluated using the Icarus material response tool.

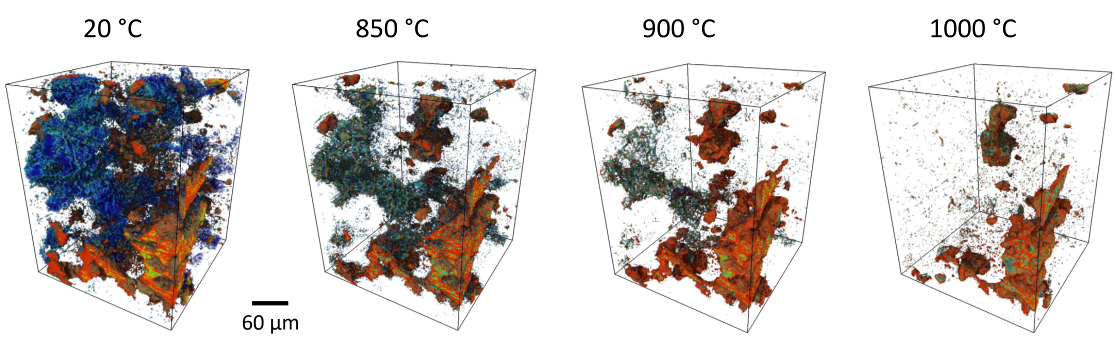

Figure 1: Progressive vaporization of troilite observed in micro-tomography reconstructions. The matrix is rendered transparent to highlight the metal grains. Blue to red color field represents increasing density.

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Development of a Melt Flow Boundary Condition in the Icarus Material Response Solver

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Abstract

The Asteroid Threat Assessment Project (ATAP) was created under the NASA Science Mission Directorate (SMD). One of the objectives of ATAP is to develop the ability to analyze the entry into the Earth's atmosphere of asteroids large enough to cause significant loss of life and devastation to the Earth [1]. These asteroids, ranging in size up to several kilometers wide, will enter the Earth's atmosphere at velocities of 12 – 30 km/s. Due to high entry velocity, and the nature of astroidal materials, material response codes applied to asteroid entry must account for effects such as surface melting, vaporization, spallation, and fragmentation.

In order to obtain experimental data for material response code model development and validation, a series of experiments were performed in 2016 and 2017 in the NASA Ames Interaction Heating Facility (IHF) arcjet [1]. Test articles made from basalt, Tamdakht meteorite, and fused silica were exposed to heating rates up to 3400 W/cm^2. More recently, a series of tests with meteorite materials were performed in the NASA Langley HYMETS facility [2]. The HYMETS facility uses a 400 kW segmented arc heater, and can produce heating rates up to 500 W/cm^2. Materials used in the HYMETS tests included basalt, quartz, the Tamdakht ordinary chondrite meteorite, and iron. The iron tests produced detailed time histories of surface and backface temperature, as well as recession rate. An example is shown in Fig. 1, that can be used for development of a melting boundary condition in a material response code.

In this study, the HYMETS test data will be used to develop and validate a melting boundary condition in the Icarus material response code [3]. The simplest implementation of a melting boundary condition is to assume that any energy flux beyond that required to raise the surface temperature to the melting point will be directed towards converting solid material to a molten state. The molten material is assumed to be immediately removed from the surface thus defining the surface recession rate. This "simple melting" boundary condition should be conservative compared to a more sophisticated melting boundary condition that would model the transport of molten material along the surface due to pressure gradients and shear forces. This study will use Icarus and the HYMETS experimental data to evaluate various melting boundary condition formulations.

Keywords: Material Response, Melting Boundary Condition, Arcjet Test Data

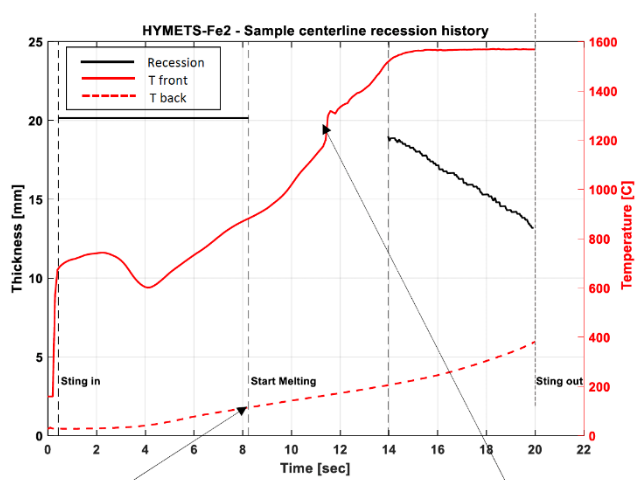

Figure 1: Temperature and surface recession time histories, HYMETS Test 2 with iron sample.

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Ablation test-case series: what about joining forces around a generic pyrolysis test-case series shared with the fire and biomass communities?

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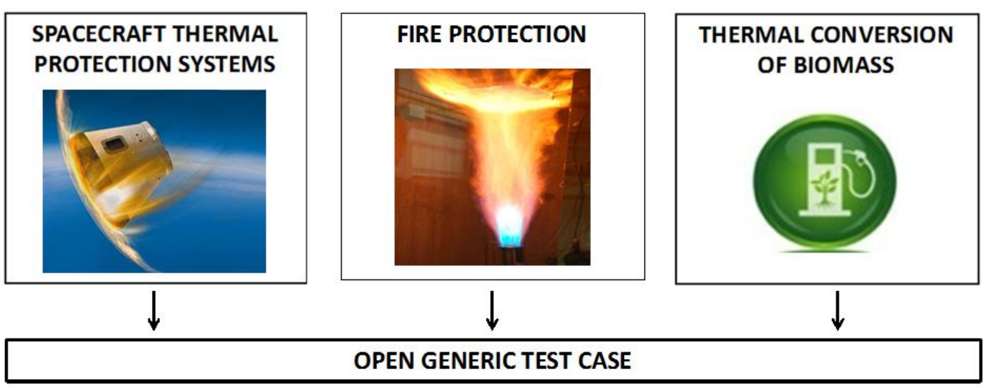
Abstract

Pyrolysis phenomena in porous media are encountered in a broad variety of high-temperature applications [1]. During the spring, a lecture series was organized at the von Karman Institute addressing three topics: I. Thermal protection systems (TPS) for spacecraft atmospheric entries, II. Fire protections, and III. Thermal conversion of biomass into biofuel. The three communities reviewed their respective fields, presenting specific workshops and test-case series, sharing good (and bad) ideas [2]. It appeared that the current scientific challenges are essentially the same, oriented towards the final long-term objective of being able to accurately predict the chemical species injected in the environment. Indeed, for all these applications, the nature of the pyrolysis gases injected in the boundary layer is key to the process studied, i.e., the boundary layer gases that interact with the hypersonic flow, the gas that sustains the flame, or the biofuel that is produced. To date, the nature of the pyrolysis gases flowing out of the materials is basically unknown. Solid pyrolysis models are just starting to become sufficiently detailed to allow us to predict the species that are produced in the pyrolysis zone. Joining forces, a generic test case series was drafted, including three cases : (1) Generic 1.0 : modeling of a thermogravimetric analysis (TGA) in 0D, (2) Generic 1.1 modeling of TGA in 3D (sample + crucible + lid / no-lid); (3) Generic 1.2 : 1D code/model comparison similar to the ablation test-case 1 of the aerospace community. A pyrolyzing numerical material for open testing (PYNOT) is also being developed. The objective of this presentation is to review the current status of this effort and open discussions.



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Numerical simulation of porous flow and ablative test case under supersonic flow conditions

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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 at atmospheric entry conditions. Volume Averaged Navier-Stokes equations (VANS) are employed to develop a universal solver (KATS-US) that solves both porous and flow domains at the same time. Numerical testing and verification is carried out through two benchmark channel flow problems. Additionally, a set of simulations of a permeable arc-jet test sample is carried out under supersonic flow conditions in order to study high velocity flow through porous materials. A qualitative assessment of shock formation, porous flow development, pressure change across the porous sample and temperature evolution throughout the porous domain is studied. Also, an ablative test case is studied under high velocity flow to assess the ablation model capability of the newly developed tool.

Keywords: Atmospheric Entry, Porous Flow, Permeability, Universal Solver, Ablation.

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A Multiphysics Phase-Field Tool to Model Ablative PICA Thermal Protection System on Atmosphere Entry Conditions

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Abstract

Phenolic Impregnated Carbon Ablator (PICA) is NASA's heritage material for ablative Thermal Protection Systems (TPS). PICA has been successfully used in the Stardust mission, with an outstanding performance during an entry on the order of 12 to 13 km/s into Earth's atmosphere, with a material recession that was considerably lower than the predicted [1]. Due to its accomplishment, PICA was utilized in the Mars Science Laboratory (MSL) probe, which successfully entered Mars' atmosphere, and it is being considered for near future missions to Mars and the Moon. Therefore, there is a large investment to increase the accuracy of the prediction capabilities to facilitate next missions. One field of interest is to understand how the PICA microstructure affects the thermal performance of the TPS. PICA is composed of dispersed carbon fibers impregnated with phenolic resin, and there are many variants to the manufacturing process that may yield a material with different properties. A multiphysics mesoscale tool is under development to aid the investigation of the PICA microstructure effects. The PICA Chemistry Utility (PICA-ChU) is an application based on the Multiphysics Object-Oriented Simulation Environment (MOOSE) framework, a c++ finite element nonlinear solver built on libmesh and PETSc [2]. The goal of this application is to represent the ablation phenomena at the microstructure of PICA by modeling the physical and chemical processes with a nano to microscale resolution. Figure 1a shows the preliminary results for a single carbon fiber oxidation, where the gas products and the microstructural evolution are quantitatively captured. The model is undergoing a verification against an analytical solution proposed by Lachaud et al. [3], which predicts the shape of the carbon fiber after oxidation under a specified set of parameters. Figure 1b represents the initial effort to verify against the aforementioned analytical solution. The results will be concluded and presented at the Ablation Workshop 2019.

Keywords: Thermal Protection System, PICA, Phase-Field, Carbon, Oxidation

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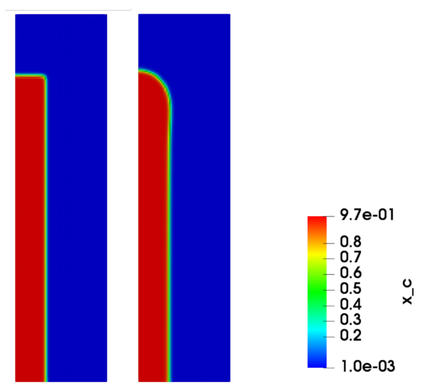
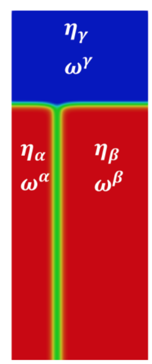


(a)



(b)

Figure 1: (a) A two-phase simulation of a single carbon that undergoes oxidation on the presence of oxygen gas. The oxidation gas products and the co-evolution of microstructure and effective properties are quantitatively tracked in the phase-field method. (b) A multiphase simulation of a carbon fiber (represented by phase α), a solid matrix (phase β), and a gas phase (phase γ). The multiphase simulation is used to verify the model against an analytical solution. The verification and other relevant results will be presented at the Ablation Workshop 2019.

Video processing for evaluation of ablative behavior of meteorite samples tested in the IHF and HyMETS Arc-Jet facilities

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Abstract

Earth is continuously colliding with fragments of asteroids and comets of various sizes which enter the Earth atmosphere at speeds ranging from 11 km/sec to 72 km/sec. Most of the fragments are about the size of a grain of sand and produce only a streak of light in the sky, but some might be large enough to penetrate deep into the atmosphere and cause damage due to blast wave, radiation, or ground impact as it happened recently with ∼19 m Chelyabinsk superbolide that fell in Russia in 2013 [1].

During the entry, the meteor is slowed down by drag and its kinetic energy is going into heat, material ablation, light and energy of ionization. Most of the meteoroids usually have a stony or metallic composition and the enormous heat formed during the entry easily melts and evaporates the surface material, thus reducing the mass. Typically, in meteor physics trajectory simulations, these phenomena are captured through two parameters: the heat of ablation and the heat transfer coefficient.

To study the phenomena of meteorite ablation, two test campaigns were recently performed at NASA Arc-jet facilities as a part of Asteroid Threat and Assessment Project (ATAP). One campaign was performed in 60 MW IHF test-facility at NASA Ames [2] and the second in 400 kW HyMETS test-facility at NASA Langley. Four different types of materials were tested: two meteorite samples - stony type H5 ordinary chondrite (Tamdakht) and an iron type IAB-MG meteorite (Campo Del Cielo) and two terrestrial analogs, Dense Flood Basalt and Fused Silica. The samples were tested at different heat flux conditions varying from 150 to 350 W/cm^2 in the HyMETS facility and around 3500 W/cm^2 in the IHF. Diagnostic methods included high speed videos, surface temperature data from pyrometers and infrared cameras, CT scan images, as well as flowfield emission from optical spectroscopy.

This study was done during an internship at NASA Ames Thermal Protection Materials Branch and will present the analysis of high speed videos captured during the IHF and HyMETS campaigns. Analysis of the videos allowed to evaluate the time-dependent cross-sectional ablation and calculate the heat of ablation values of each of the test samples. Additionally, these analyses can provide data for validation of multi-dimensional ablation simulations. Illustration of the ablation behavior of Tamdakht meteorite sample is presented in Figure 1. As well, it will be shown that using a setup of high speed and even regular HD side-view camera, appropriate filter and exposure time accompanied with relatively simple image processing algorithm a convenient method can be developed for monitoring the ablation behavior of various samples in Arc-Jet facilities.

Keywords: Meteorites, Ablation, Arc-Jet,Video processing

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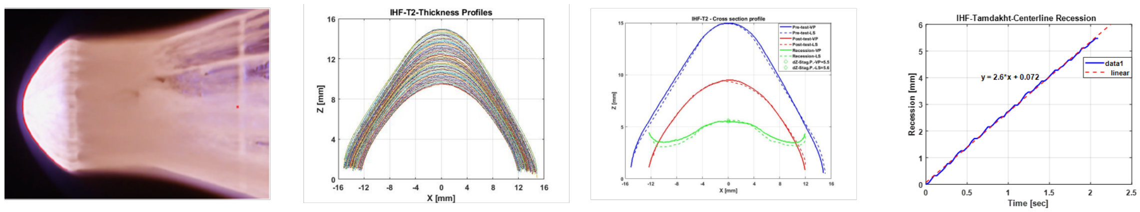

Figure 1: Ablative behavior of meteorite Tamdakht sample in the IHF.

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Strain-Dependent Analysis of Conductivity in Fibrous Insulation Materials

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Abstract

Fibrous insulation materials are often used in thermal protection system applications to insulate the vehicle from the thermal environment of re-entry and hypersonic flow. This insulating effect can take many forms, such as through out-gassing of chemical reactants and phase change phenomenon; however, the primary effect comes from the low thermal conductivity of these materials. The conductivity is a function of not only the temperature, environmental pressure and composition of the material, but also of the internal geometry. This internal geometry affects radiation exchange between fibers as well as conduction paths between the fibers and internal gas. Changing the geometry will therefore change the conductivity characteristics, which can happen under strain of the material. This strain can be induced by mechanical stressing of the material in re-entry or through folding and stretching of the material, such as in HIAD systems. Thus, this work will explore the characterization of conductivity in these materials under various strains. The experimental apparatus used will be a cut-bar metering apparatus, with electronically actuated motors, LVIT, and force sensors to capture the stress and strain of the material along with conductivity. This analysis will be coupled with previous work to model the independent modes of conductivity in the material.

Keywords: Heat Transfer, Conductivity, Fibrous Insulation, Stress, Strain, Cylinder

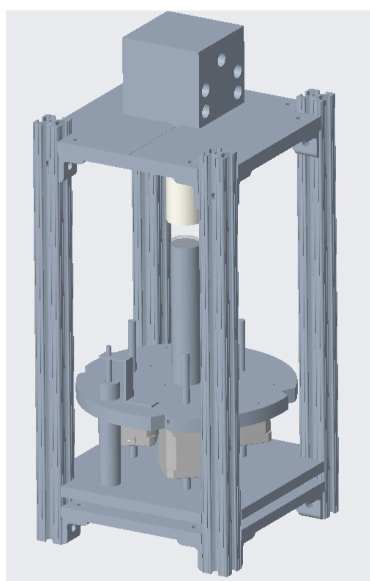

Figure 1: Rendering of modified metering bar apparatus

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Finite-rate air-carbon ablation model

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Abstract

The goal of this work is to develop a finite rate air-carbon ablation model that can be used in Computational Fluid Dynamics (CFD) to accurately simulate ablation experiments. Measurements made in plasma flow facilities, such as the surface heat flux and recession rate are the result of many coupled processes. It is difficult to fully parameterize models using such data. Instead, we use experimental data from molecular beam (MB) experiments to develop a finite rate air-carbon ablation model. Poovathingal et al. [1] and Gopalan et al. [2] developed finite-rate models for oxidation based on MB experiments. We modify the oxidation model by Poovathingal et al. so that the model agrees with new experimental data. We also add nitridation to the model using the MB data of Murray et al. [3], oxidation by O_2 using MB data from Edel et al. [4], and oxidation by CO and CO_2 using flow-tube reactor data from Panerai et al. [5]. Murray et al., in their work on carbon nitridation, concluded that the reaction probability of CN production has an Arrhenius temperature dependence with an activation energy of 207 kJ/mol. However, we find that an effective activation energy of 57 kJ/mol, along with N-atom adsorption selectivity of 0.01 gives good agreement with a wide range of experimental data. Model parameters include the active site density on the surface, the pressure of the gas above the surface and the reaction constants. We present zero-dimensional (ZeroD) simulations of the model by deriving a steady state solution to the set of time-dependent ordinary differential equations. The model can be used to run ZeroD simulations of gaseous mixtures, given the gas composition and the pressure, both in steady state mode and transient mode.

For example, Figure 1 shows the probability of CN formation as a function of temperature comparing the model with various experimental data sets. The black line is the CN probability predicted by model at 4.75e-05 Pa representative of a molecular beam and can be compared with the experimental data (represented by black dots) from Zhang et al.[6]. The blue line is the model prediction at 1600 Pa, representative of the partial pressure of N at the carbon surface at VKI plasmatron conditions and can be compared with the plasmatron experimental data (blue dots) from Helber et al. [7]. We see that the new model agrees reasonably with the experimental data across various range of pressures. The Park model (green line) gives a CN probability that is significantly higher than the data. The red line is the model prediction at 4.75e-05 Pa when an activation energy (E_a) of 207 kJ/mol is used for CN production.

In the final work, we will present simulations for gaseous mixtures of different compositions and discuss the effect of temperature on the time taken to reach the steady state, the effect of pressure on the steady state and competition between nitridation and oxidation on the carbon surface.

Keywords: Finite rate model, nitridation, oxidation

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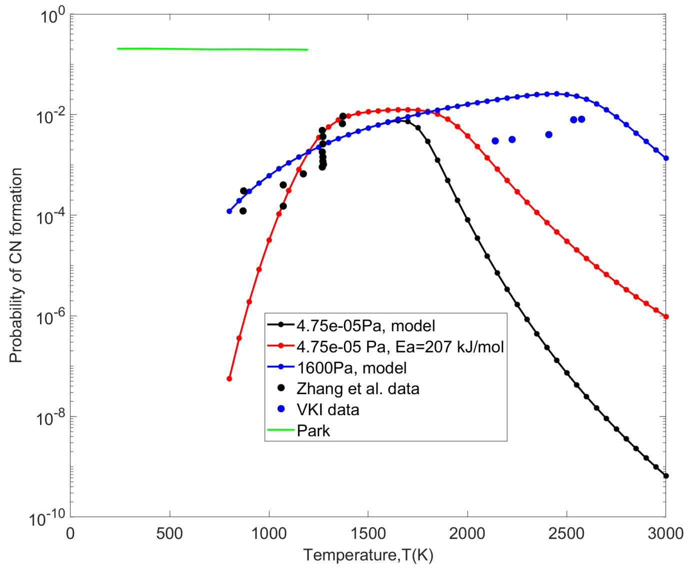

Figure 1: Probability of CN formation as a function of surface temperature for various pressures

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Decomposition of Heat Shield Silicones Under Atomic Oxygen Bombardment

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Abstract

Silicone materials on heat shields used in the presence of atomic oxygen may form a passivating SiO_2 layer that slows the decomposition of the silicone material itself or the substrate on which it is applied. We have initiated a study of two silicone materials, Avantor Nusil's CV-1144-0, and Momentive Perfomance Materials' RTV-560, which are deployed as heat shield coatings and binding agents, respectively. Understanding the oxidation and mass loss rates of these materials as they are heated under atomic-oxygen bombardment will thus provide valuable data for ablation models. Using a unique atomic-oxygen pulsed beam with ~5 eV energy as well as a heated quartz crystal microbalance (QCM) apparatus from Colnatec, Inc., we have investigated the mass loss as a function of temperature during atomic-oxygen bombardment. Preliminary results after atomic-oxygen exposure show significant loss of surface carbon for exposures at both room temperature and 300°C, along with XPS peaks representing formation of SiO_2 at both temperatures. Additionally, cracks appear after O-atom exposure, suggesting that the volume change associated with the formation of an SiO_2 layer results in stress-induced cracking. Mass-loss measurements show an initial increase in mass, followed by subsequent mass loss. The overall mass loss at room temperature is negligible compared to the mass loss of a hydrocarbon polymer, presumably because of the passivating SiO_2 layer that is formed on a silicone material. We will report a detailed study of the relationship between mass-loss rate and temperature (up to 600 °C) with and without atomic-oxygen bombardment.

Keywords: Silicone, thermal decomposition, atomic oxygen, mass loss

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Heatshield Erosion due to Dust Particle Impacts on the Schiaparelli Capsule During Martian Entry

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Abstract

On October 2016, a capsule known as Schiaparelli, part of the European Space Agency (ESA) ExoMars mission, entered the Martian atmosphere. Measurements taken during the Schiaparelli descent will be used to validate computational models used to design the thermal protection system (TPS) of future Mars missions [1]. One of the unique features of Schiaparelli entry was the possibility of a major dust storm occurring during the entry. Major dust storms are unpredictable but more likely during the Northern Autumn timeframe. In 2001, for example, regional dust storms merged into a global dust storm that blanketed much of the planet. Even though Schiaparelli did not enter during a major dust storm, future Mars missions will have to account for the possibility of dust erosion (depending on the time of year) when estimating the thickness of the TPS. Because weight is always a critical factor in designing entry vehicles, accurate assessment of dust erosion is necessary to avoid over-design of the TPS.

This study will present computational results of heatshield erosion due to dust particle impacts on the Schiaparelli capsule if it had encountered a dust storm during entry. An uncoupled approach will be used where the particle trajectories are assumed to not impact the shock layer flow. The DPLR CFD code [2] will be used to compute Navier-Stokes flow solutions at 11 points along the entry trajectory. The particle trajectories through the shock layer are calculated by solving a set of coupled ordinary differential equations that make use of the underlying CFD solutions. The particle calculations continue until either the particle strikes the surface of the heatshield, miss the heatshield entirely, or disappear due to surface vaporization. Figure 1 shows a sample calculation where the particle velocity, shown in the circles, of 1-micron diameter dust particles decreases as the particles travel through the shock layer at the 40 km trajectory point. The particle trajectories begin to bend upward due to the effect of the underlying flow velocity.

Once the particle trajectory computations are complete, the information is passed to the Icarus material response code [3]. A dust erosion boundary condition has recently been added to Icarus that computes surface recession due to dust particle impacts. The initial implementation of this boundary condition uses the damage model of Papadopoulos, Tauber, and Chang [4] that is based on Apollo- and Shuttle-era experimental data. Under this model, the heatshield erosion is a function of the number density, velocity, and diameter of the particles at the point of impact. In addition to this model, more recent erosion models will also be implemented into the Icarus material response solver and comparisons between the models will be performed.

Keywords: Thermal Protection Systems, Planetary Entry, Dust Erosion

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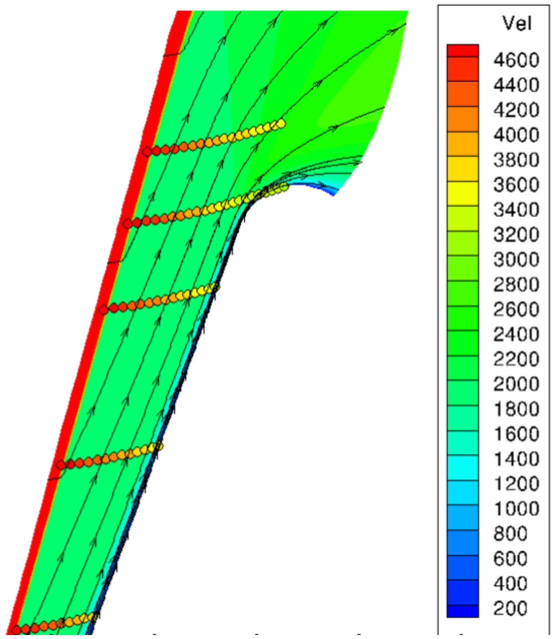

Figure 1: 1-micron diameter dust particle trajectories and velocity magnitude through the shock layer, 40 km trajectory point.

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Overview of modeling micro-meteoroid and orbital debris impact cavity growth

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Abstract

Missions which require spacecraft to spend extended time in low earth orbit are particularly susceptible impacts by micro-meteoroids or orbital debris (MMOD). This risk, coupled with the tight planetary protection requirements imposed on sample return missions, drives a need to better understand failure mechanisms of thermal protection systems. The aim of this work is to gain an understanding of MMOD impact cavity dynamics during atmospheric re-entry through computational modeling. MMODs that can pose a significant threat can travel at velocities between 7-60km/s, having mass distributions ranging from 1μg-10g, and densities between 0.1-10g/cm^3 [1], where the corresponding kinetic energy bounds are 2.45×10^{-5}J and 18J. Furthermore, impacts can occur at any point on the heatshield or backshell, and at any angle. Because of these wide ranges of possible collision characteristics, it intractable to study every combination of conditions to insure spacecraft reliability. As a consequence, it is necessary to understand what the dominant scales of the problem are so that ranges of cavity sizes and shapes can be classified and appropriate predictions can be made about failure. However, a necessary first step to do this is to develop, test, and verify the computational methods on a generic test case. This work addresses the first step in computational prediction of cavity growth, in that a generic (corresponding to an average severity) impact cavity is studied with the current state-of-the-art tools. First, for an initial cavity shape, the fluid dynamic behavior is studied. The overall heating augmentation is determined as well as the 3-dimensional heat flux, and surface pressure distribution. The boundary layer edge properties are also computed in order to obtain the effective heat transfer coefficient to the solid surface. The US3D [2] computational fluid dynamics code is used for this analysis and grid interpolation routines are leveraged for efficiency. The 3D aerothermal boundary condition, obtained from CFD, is then applied to a material response solver, Icarus [3]. Then the heat conduction in an orthotropic material is studied as well as pyrolysis gas transport. Of interest is the effect that a pressure gradient due to geometric non-uniformity has on driving porous gas flow, based on Darcy's Law, and the subsequent heating, decomposition, and charring that occurs. Finally, a thermoelastic module in Icarus [4] is used for studying thermal stresses near the cavity walls. This can provide insight into non-thermal failure modes e.g. spallation, delamination, crack formation, which will not be addressed in this work but may become necessary considerations for future studies. The last stage of this work is to provide a preliminary assessment of how much each of the mechanisms mentioned above is affected by the cavity presence, and how these changes may contribute to failure.

Not captured is the shape change the cavity undergoes and the dynamically coupled interaction between the latter and the aerothermal environment.

In summary, a generic cavity shape will be chosen based on impact scenario probability distributions, and the aerothermal, thermal and structural response will be studied in an uncoupled manner. Preliminary assessment of dominant physical mechanisms will be made.

Keywords: Thermal Protection Systems, Heat Transfer, Mass Transfer, Aerothermodynamics, Thermoelasticity, MMOD

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Implementation and verification of a mesh motion scheme using radial basis functions in the Icarus material response code

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Abstract

In order to model macro-scale ablation with high-fidelity, it is necessary to accurately capture the shape change a material undergoes due to mass removal at the surface. This requires the implementation of a mesh-motion scheme as well as a recast of the governing equations into a moving frame of reference.

In this work, radial-basis functions are used as an algorithm to move the mesh, in the Icarus material response code [1]. This method presents some advantages over the tension and torsional spring analogy methods as well as the PDE based methods such as the linear elastic analogy, because it does not require knowledge of the grid connectivity. This makes it well suited for use on unstructured, arbitrary elements without requiring the solution to a system of equations at every mesh point. The volume-point interpolation function is of the form

$$s(\mathbf{r}) = \sum_{i=1}^{i=N} \alpha_i \phi(\|\mathbf{r} - \mathbf{r}_i\|), \tag{1}$$

where the motion of the volume points is determined by the function $s(\mathbf{r})$ evaluated at location $\mathbf{r}$ (control points). Here, ϕ is the basis function whose arguments are the distances between the control points, $\mathbf{r}$, and each volume point $\mathbf{r}_i$, and α_i are the interpolation coefficients to be found such that the solution is recovered exactly at the control points. This algorithm costs N_{cp}^3 for the solve and $N_{cp} \times N_{vp}$ for the update because it requires the solution to a linear system of size $N_{cp} \times N_{vp}$, where N_{cp} and N_{vp} are the number of control points and volume points respectively. For large mesh sizes this may become undesirably expensive however, data reduction algorithms can be used to significantly reduce the cost of each solve [2]. This method is favorable for fluid-structure interaction problems on multi-block, unstructured grids, which will be a requirement for high-fidelity cavity shape change studies with couple fluid-solid interaction [3].

Once the method is implemented, the finite volume formulation of the governing equations must be re-derived to account for a time-varying control volume. In practice this means that the artificial flux generated by the movement of the mesh must be countered by an equal and opposite flux such that the conserved variables remain unchanged by movement of the grid. Furthermore, a source term is introduced which originates from the time-derivative of the differential volumes. These terms are included in the explicit update to an otherwise implicit time-integration scheme. A series of verification tests are carried out to insure strict conservatism is maintained and gradients of primitive variables are preserved, as well as correct implementation of mesh motion algorithm itself. Finally, this method will be used for capturing shape change of a moderately complex geometry i.e. an ablating cavity, and its suitability for this type of problem will be assessed.

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Modeling bourbon barrels

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Abstract

As opposed to wine barrels, which are usually toasted, bourbon barrels are legally required to be charred in order to be qualified to age bourbon. The charring process is known to both influence the color and the flavor during the aging process. The heat caramelizes the natural sugars of the oak, and creates some of the most interesting flavors of finished product. The process also opens up the wood by modifying the porosity at the surface, thus allowing the liquid to penetrate deeper into the wood. The flavor profile of bourbon is known to come from three different sources: the mash bill (type of grains), the fermenting yeast, and the oak barrel. It is estimated that the barrel contributes to about 50-70% of the flavor profile. However, between these three factors, controlling the flavor obtained from the barrel remains difficult. Part of this aspect comes from the variability of the barrel, which might have been constructed from different part of a tree, different trees altogether, or trees harvested in different forests. But the difficulty also comes from the variabilities within the wood itself, where the grain is distributed non-uniformly, or can even have impurities. Both of these variabilities ? large scale and small scale ? have significant effects on the tasting profile of the bourbon, where a barrel with the same properties, used to aged the same liquid in the same location, will give a widely different results. Nowadays, the good barrels ? the so-called honey barrels ? are often used to produces the top of the line limited bourbon releases, and the regular ones are usually mixed in large batches to produce main stream products. The current work aims at modeling the heat transfer, the pyrolysis and the charring of the oak staves during fabrication. This is achieved by using advanced material response tools that can model the heat propagation, the pyrolysis of the wood and the charring process of a material subjected to a heat flux.

Keywords: Bourbon, thermal response, toasting, charring, chemical decomposition

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

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Abstract

Spallation is a form of ablation where the material mitigates the high heat rates through particle ejections. The ejections of particles accelerate the material recession and the presence of them in the flow field tend to change the surface heating rates due to their chemical interactions.

To quantify and qualify the behavior of ejected particles, spallation experiments were conducted at NASA Langley's HYMETS arc-jet facility [1]. High-speed imagery and particle tracking velocimetry algorithm 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 essential to know that the initial state of the spalled particles to evaluate the mass loss due to spallation, and 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. A data-driven adaptive technique [4] is implemented to reconstruct the numerical trajectories that match with the experimental ones.

Keywords: Spallation, Ablation, Arc-jet, Thermal protection system

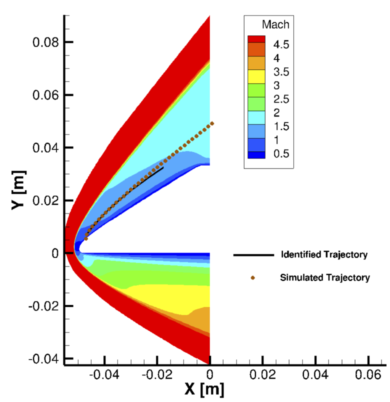

Figure 1: Reconstructed Numerical Trajectory

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Fully coupled material-environment simulation of a Simoun plasma wedge test on a conformable C/P with PATO.

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Abstract

Porous carbon/phenolic (C/P) conformable ablators are being developed by Ariane Group as an extension of the ASTERM charring ablator family [1]. They are foreseen as candidates for future Mars missions of the European Space Agency. To reproduce typical environments met during Mars entry, samples have been tested at Mach 5 in wedge configuration in one of the plasma wind tunnel of Ariane Group, namely Simoun (fig. 1).

The conformable C/P is similar to denser original ASTERM composites; although a 50K temperature jump is observed at the bondline right at the start of an arc jet test. This phenomenon has already been reported - in a lesser extend though - for PICA during MSL entry (in MEDLI) and for some arc jet tests carried out at NASA Ames. The most plausible explanation is that hot boundary layer gases suddenly fill porous materials at the start of the tests.

To better understand and model the coupling between external pressure and internal gas flow, a fully coupled material-environment approach has been developed in PATO. A Darcy model (type 2) is used in the porous material. The rhoCentralFoam solver of OpenFOAM has been integrated and explicitly coupled with PATO to resolve the shock and flow field. It is based on a compressible Kurganov Tadmor scheme. Gas chemistry is considered frozen from the outlet of the nozzle. An analysis of the gas flow within the ablator will be presented. In Figure 2, the pressure field is presented at time 0.001 seconds. As we are submitting this abstract, computations are running to reach 1 minute by September 2019.

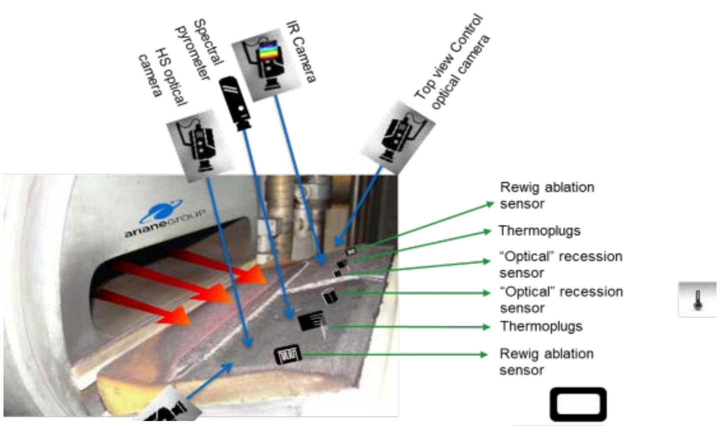

Fig1: Simoun arc jet and instrumentation in wedge configuration

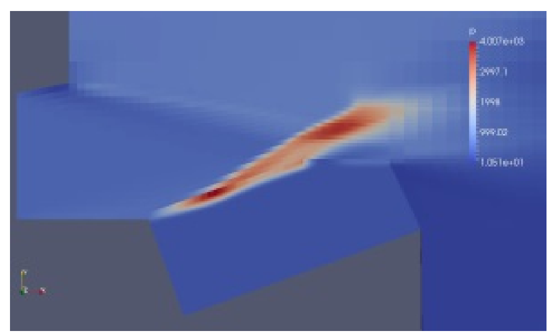

Fig2: Coupled simulation in PATO (t=0.001s)

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Computational Analysis of Thermal Protection System with Embedded Vascular Network

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Abstract

Micrometeoroids and Orbital Debris are a significant problem in Low Earth Orbit (LEO) as humans continue to send satellites to space. Over the next hundred years, the amount of orbital debris is expected to increase exponentially. This is a danger to spacecraft, as the increased amount of debris results in a higher risk of collision and subsequent damage. All spacecraft are at risk, but re-entry vehicles face unique challenges because any damage to the thermal protection system will impact the survivability of the vehicle when it enters the atmosphere. Research by Ng has shown that these damages, when exposed to heating in a hypersonic flow, do increase the temperature seen at the bondline for insulating materials [1]. This risk is especially significant for missions that seek to have high reliability, such as sample return missions and human missions.

One possible solution to increasing the reliability of the vehicles that are especially susceptible to damage from orbital debris is to include a self-healing mechanism in the thermal protection system. A vascular self- healing system was chosen because MMOD damage can result in a significant loss of material in the TPS, and a vascular mechanism would enable sufficient healing material to be delivered to the damage site.

Previous research has looked at characterizing the depth that the vascular system must be placed in order to adequately protect the TPS from damage. This depth is referred to as the critical depth and is the through-the-thickness depth in the thermal protection system at which the remaining thermal protection system material is not sufficient for successful entry [2]. Additionally, the self-healing fluid will have to cure at the damage site in order to protect the TPS during entry conditions. If the damage does not reach the self-healing system, then it is desirable that the self-healing material does not cure and can be reused. The location of the vascular system in the TPS will then inform the types of materials that can be chosen as self-healing fluids in this system.

These considerations will be examined using various heat conduction tools, assuming one-, two- and three-dimension heat transfer. The material is assumed to be LI-2200, which is a reusable ceramic insulating material. The tubes in the material will be modeled as voids in the system, with internal surface to surface radiation included.

Results will show placement restrictions on the tubes such that they dont impact the bulk TPS properties as well as restrictions on the self-healing material such that is survives multiple entry heat pulses. The results from these models will then inform the test articles built for testing in a radiant heater facility at NASA Ames Research Center.

Keywords: Heat Transfer, Thermal Protection Systems, MMOD, Self-Healing Materials

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Modeling Carbon fiber oxidation under high temperature by ReaxFF based molecular dynamics simulation

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Abstract

As a polymer-based ablator, the Phenolic Impregnated Carbon Ablator (PICA) material, a composite made of a resin matrix and carbon fiber, is widely used in Thermal Protection Systems (TPS) to protect space vehicles during atmospheric re-entry. Oxygen diffuses into the PICA and reacts with the carbon fibers during the pyrolysis and ablation processes. The purpose of this study is to model and investigate the surface chemical reactions and structural changes of carbon fibers under the extreme conditions like high temperature. The carbon fiber model is generated by a method developed by Desai et al.[1], which combines kinetic Monte Carlo and molecular dynamics (MD) techniques. MD simulations based on a reactive-force-field (ReaxFF) potential are performed to investigate the oxidation in this carbon fiber model at high temperature. The influences of the oxygen concentration and the temperature to carbon fiber oxidation are characterized. The preliminary results of this simulation show the carbon fiber oxidation exhibits a temperature dependence and the major product during the reaction is carbon monoxide, which is in good agreement with other simulations.

Keywords: Ablation, Carbon fiber, Phenolic Impregnator Carbon Ablator, Molecular Dynamics, ReaxFF

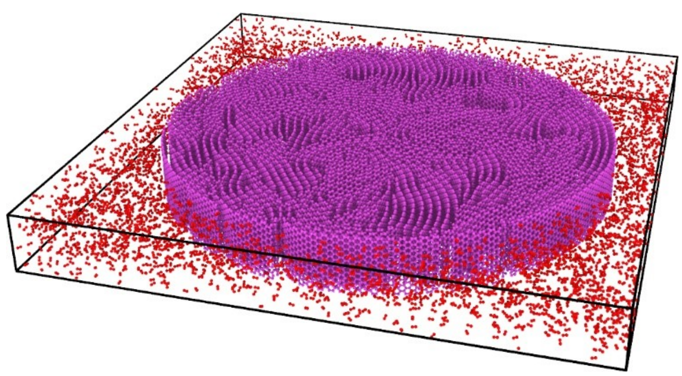

Figure 1: Side view of the initial state of carbon fiber simulation, red atoms are oxygen atoms and pink atoms are carbon atoms.

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Surface Properties on Thermal Protection System Microstructure at Flight Relevant Conditions

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Abstract

New planetary missions will require higher reliability ablative TPS to handle high heating rates and shear loads while providing the necessary thermal protection for the interior of the vehicle. For example, due to the small margin for error and critical aerothermal environment, higher fidelity modeling will be needed for missions including Mars Sample Return. During the ablation process, thermal stresses and traction forces combined with oxidation could affect the structural integrity of the TPS resulting in failure. For example, spallation may cause unwanted surface modifications and faster carbon ablation than anticipated, and thus may lead to the failure of the TPS [1]. In this work, hypersonic boundary layer flow is simulated over TPS microstructures using the Direct Simulation Monte Carlo (DSMC) method where boundary layer profiles are extracted from a CFD simulation of the Stardust capsule.

FiberGen [2] is used to create a microstructure representing a standard Fiberform bundle. Fiberform has average porosities higher than 85% where their microstructure is characterized by fibers preferentially aligned at about ±15° perpendicular to the direction of compression where fibers are mostly parallel to the ablation surface [3]. Different bundles with varying porosities are created since the stress distribution within the microstructure is governed by the material porosity [4]. Previous work included simulating boundary layer flow over a single microstructure at one Stardust altitude [5]. The current work simulates boundary layer flow over multiple microstructures at two Stardust altitudes with improved statistics. Significantly, the current work illustrates the capability of getting the distribution of surface properties of the fiber bundle and the ability of isolating individual fibers for use in thermo-structural analysis [6]. Preliminary results of the heat flux are shown below for two instances of the Stardust reentry in Figure 1. One can see that the heat flux for the fibers closer to the boundary layer is higher for the lower altitude case as expected. The distribution of the heat flux for the fiber bundle is shown in the left of Figure 2 which will be useful in selecting which fibers will fail for thermo-structural analysis. Lastly, the capability of pulling out a specific fiber and plotting its surface properties is demonstrated on the right of Figure 2.

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

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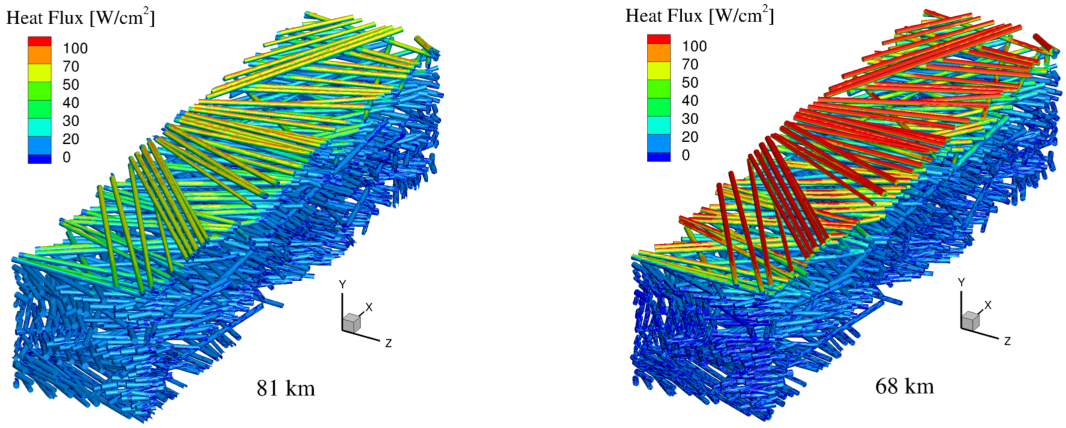

Figure 1: Heat flux contours corresponding to Stardust boundary layer conditions at two trajectory points

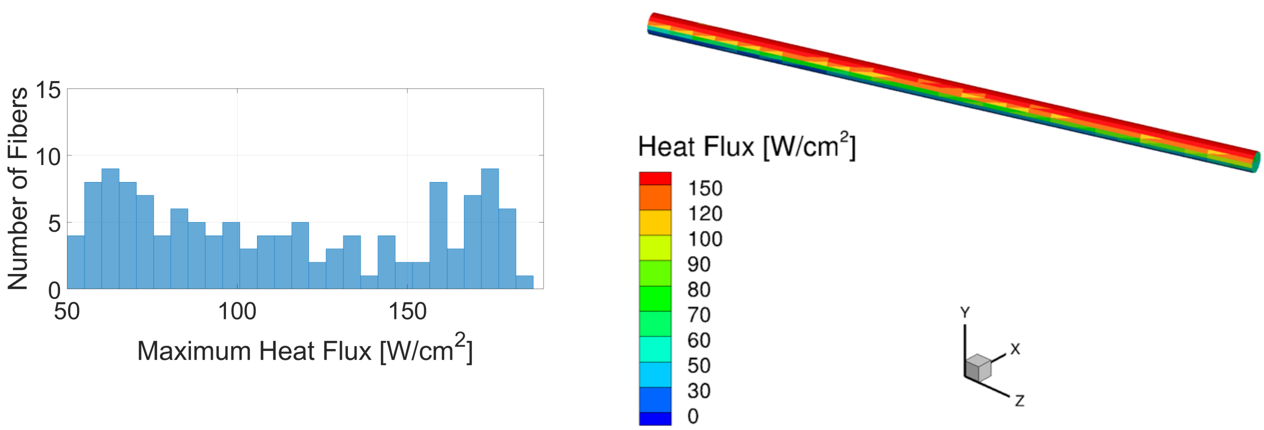

Figure 2: (Left) Histogram of individual fiber properties and (Right) Capability to post-process individual fibers

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Bayesian Inference and the Effects of Varying Uncertainty Models in Charring Ablator Calibration and Uncertainty Quantification Problems

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Abstract

The Mars Science Laboratory vehicle utilized a heat shield constructed from NASA's Phenolic-Impregnated Carbon Ablator material to protect the main structure from the high enthalpy environment encountered during hypersonic atmospheric entry. During the vehicle's descent through Martian atmosphere, multiple thermocouples embedded within the heat shield captured in-depth material temperature data that allow for studies to be conducted on current material response reconstruction tools. In the present work, material temperature data obtained from thermocouples within the MISP-4 plug are utilized in the calibration of TACOT model parameters in conjunction with NASA's Porous material Analysis Toolbox (PATO) through Bayesian inference where uncertainty due to parametric, modeling, and experimental sources is simultaneously quantified. Prior to the study, a sensitivity analysis is performed through computation of the robust Sobol indices in an effort to study the relationship between input space and model response and to reduce the dimensionality of the statistical inverse problem. The Bayesian inference methodology necessitates an a-priori choice to be made for the uncertainty model for which numerous possibilities are available. Across most works, however, only basic additive or multiplicative models are utilized with pre-defined magnitudes of uncertainty based on a-priori knowledge or to-be-calibrated multipliers of static covariance matrix structures. The present effort explores the effects of informed uncertainty models, ones with temporal dependence that are simultaneously calibrated through Bayesian inference, on calibrated results for parameters that make up the uncertain input space.

Keywords: Bayesian Inference, Sensitivity Analysis, Calibration, Uncertainty Quantification, Charring, Ablator, PICA, TACOT, PATO, Mars Science Laboratory, MSL

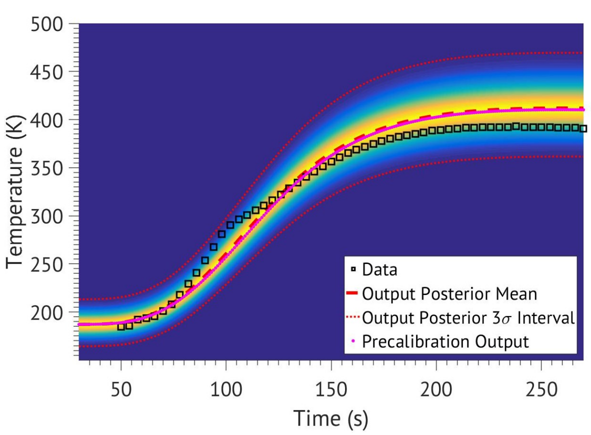

Figure 1: Results using a scalar, temporal and spatial independent multiplicative error uncertainty model for TC-3 of MISP-4 plug.

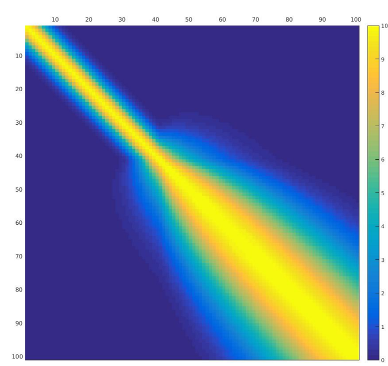

Figure 2: Realization of one of the uncertainty covariance matrix structures with temporal correlation in this study.

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Title:

A Testing and Evaluation Facilities Framework to Develop Leading Edge Materials for Application in High Speed Gas Flows

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Abstract:

The development of advanced thermal protection system (TPS) materials are needed for use in high speed aerospace vehicles. However, the relevant land based testing and evaluation national infrastructure that simulates certain critical aspects of the relevant extreme flight environment are a limited resource that will not sustain high volume routine testing to screen materials nor should they be given the limited materials characterization available during testing. Thus, it is evident that a testing and evaluation framework for understanding TPS material thermal response under relevant extreme environments is needed that incorporates the different test conditions available using national and academic test facilities that are currently available prior to arc heaters testing. The framework of national land based testing would consider a progression of test conditions available across several land based test facilities that allow for the materials response and characterization to be analyzed and thus accelerate the materials development prior to arc heater testing. The test facility must first deliver high enthalpy gas flow that will result in an increase in the temperature of the material that is high enough to promote thermodynamically favorable gas to surface reaction chemistries. The same or different test facility must then allow for the delivery of high temperature gas species relevant to the application environment. Lastly, the test facility should test the materials as a function of high temperature gas pressure. An evaluation of ultra-high temperature ceramics for proposed leading edge environment applications have been tested and evaluated using a number of high enthalpy land based test facilities, such as combustion gas torch heater, plasma torch heater, solar radiation furnace, and arc jet heaters, and will be presented as a case study to illustrate this proposed national testing and evaluation framework.

Efficient sticking of crystalline Si nanospheres via phase-transition plasticity

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Abstract

Classical molecular dynamics simulations considering a 5 nm in radius H-passivated Si nanosphere that impacts with relatively low energies onto a H-passivated Si substrate reveal a transition between two fundamental collision modes. At impacting speeds of less than ∼1000 m/s *particle-reflection* dominates. At increased speeds the partial onset in the nanosphere of a β-tin phase on the approach followed by *a*-Si phase on the recoil is an efficient dissipative route that promotes *particle capture*. In spite of significant deformation, the integrity of the deposited nanosphere is retained. Our result explains the efficient fabrication of nanoparticulate films by hypersonic impaction, where the nanoparticle impact velocities equal 1000–2000 m/s [1]. We further relate these results to the molecular dynamics description for the response of crystalline Si nanospheres for various uniaxial compression levels [2]. The behavior at low compressions closely resembles the Hertzian predictions. At higher compressions the creation of a new β-tin phase in the particle core leads to (i) volumetric changes (ii) an increase in elastic moduli, and (iii) significant hardening. Further, (iv) a reversible character of the transformation is obtained with molecular dynamics simulations. The agreement of (i)–(iv) with recent experimental findings challenges the current exclusive view of a dislocation plasticity response in somewhat larger nanoparticles. The phase-transition path should dominate in ultra-small structures, where dislocation activity is prohibited.

Keywords: Molecular Dynamics, nanoparticle collisions, hypersonic impaction

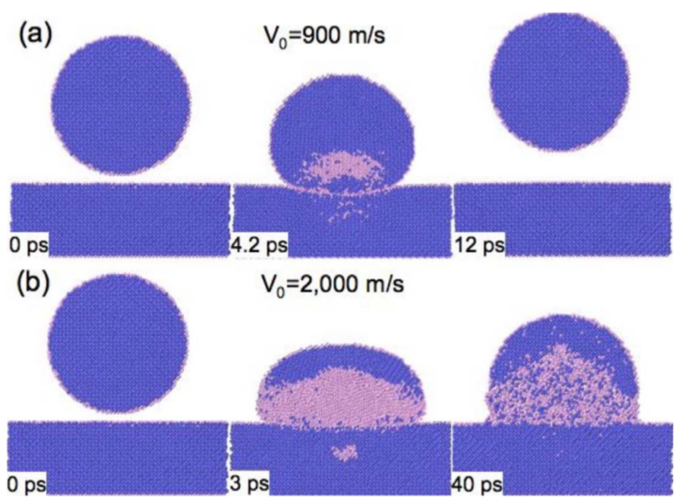

Figure 1: MD simulations of H-passivated Si nano- sphere impacting onto a H-passivated Si substrate show two colli- sion modes: (a) reflection and (b) capture. The middle frames show the maximum penetration instant. Only cross sectional views are shown and H atoms are not represented. The color code carries the local PE with blue (gray) and pink (light gray) representing atoms with PE absolute values larger and smaller than 4.4 eV/atom, respectively. Ref. [1].

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Determination of aerothermal environment and ablator material response using inverse methods

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Abstract

The Mars Science Laboratory (MSL) was protected during its Mars atmospheric entry by an instrumented heatshield that used NASA's Phenolic Impregnated Carbon Ablator (PICA) [1]. PICA is a lightweight carbon fiber/polymeric resin material that offers excellent performance in protecting probes during planetary entry. The Mars Entry Descent and Landing Instrument (MEDLI) suite on MSL offers unique in-flight validation data for models of atmospheric entry and material response.

MEDLI recorded, among other things, time-resolved in-depth temperature data of PICA using thermocouple sensors arranged in MEDLI Integrated Sensor Plugs (MISPs). These measurements have been widely used in literature as a validation benchmark for state-of-the-art ablation codes [2,3]. The objective of this work is to perform an inverse estimate of the MSL heatshield aerothermal environment and material response during Mars entry from the flight data. The Porous material Analysis Toolbox based on OpenFOAM (PATO) software [4,5,6] is used to compute the material response. PATO models PICA ablation 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. Thermodynamic and chemistry properties are computed using the Mutation++ library [7].

Parameter estimation and the inverse problem are handled by the DAKOTA optimization library [8], which is coupled with PATO. A multi-objective genetic algorithm and a trust-region method for nonlinear least squares are used to estimate key uncertain material parameters which influence the material response model.

We follow the strategy of Mahzari et al [2] by first using a thermocouple driver approach to estimate uncertain parameters in the material model. In this case, the temperature, obtained from the flight data, is imposed at the location of the shallowest MISP thermocouple. Then, the aerothermal environments (i.e surface temperature and heat flux) at the probes are estimated by fitting to the in-depth measured thermocouple response from the flight measurements. This work represents an important milestone toward the development of validated predictive capabilities for designing thermal protection systems for planetary probes.

Keywords: Mars Science Laboratory, Heatshield, Porous media, Inverse methods, Ablation, Pyrolysis

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Micro-scale artificial weave generation capabilities for TPS material modeling

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Abstract

Thermal Protection System (TPS) modeling requires accurate representation and prediction of the thermomechanical behavior of ablative materials. State-of-the-art TPS materials such as Phenolic Impregnated Carbon Ablator (PICA) have a proven flight record and demonstrate exceptional capabilities for handling extreme aerothermal heating conditions. The constant push for lightweight materials that are flexible in their design and performance, and hence allow for a wide range of mission profiles, has led NASA over the past years to develop its Heatshield for Extreme Entry Environment Technology (HEEET). HEEET is based primarily on a dual-layer woven carbon fiber architecture and the technology has successfully been tested in arc-jet facilities [1]. These recent developments have sparked interest in the accurate micro-scale modeling of composite weave architectures, to predict the structural response of macro-scale heatshields upon atmospheric entry. This effort can be extended to incorporate in-depth failure mechanics analyses as a result of local thermal gradients or high-velocity particle impact. This work presents the preliminary stages of the design tool, an example of which is illustrated in Fig. 1. The modularity in which weave patterns are generated is shown. The underlying physics to stretch the unit cells into shape, i.e. tension, bending, contact and damping, is explained in detail.

Keywords: Weave, Carbon Fiber, Unit Cell, Contact Theory

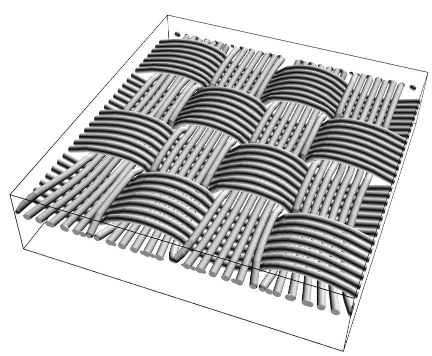

Figure 1: Conceptual design of an artificial carbon fiber weave using PuMA for visualization [2].

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Progress towards modeling the ablation response of NuSil-coated PICA

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Abstract

The Mars Science Laboratory (MSL) Entry, Descent and Landing Instrumentation (MEDLI_1) collected the first detailed in-flight data used by the ablation community to validate physics-based models for the response of the Phenolic Impregnated Carbon Ablator (PICA) material [1-4]. A follow-up instrumentation suite, MEDLI_2, is being planned for the upcoming Mars 2020 mission [5] motivated by the large scientific impact of MEDLI_1. Recent analyses performed as part of MEDLI_2 development draw the attention to significant effects of NuSil, a protective coating to the aerothermal response of PICA. To mitigate the spread of phenolic dust from PICA, NuSil was applied to the entire MSL heatshield, including the MEDLI plugs. NuSil is a space grade designation of the siloxane copolymer, primarily used to protect against atomic oxygen erosion in Low Earth Orbit (LEO) environment. NuSil effects are currently neglected in PICA ablation models. Ground testing of PICA-NuSil (PICA-N) models all exhibited surface temperature jumps of the order of 150 K due to oxide scale formation and subsequent NuSil burn-off. It is therefore critical to include a model for the material response due to NuSil coating in ongoing code development and validation efforts. Tests have been conducted at the HyMETS facility to screen the response of PICA-N and gather detailed data on its behavior. In this work, we present progress toward formulating a high-fidelity material response model for PICA-N in the Porous material Analysis Toolbox based on OpenFOAM (PATO) software [6-7]. First, the surface mass balance formulation for multi-elemental composition at the wall is described. Then, the material response simulations of a 200 micron layer of NuSil on top of PICA is presented. Finally, PATO modeling results are compared to the HyMETS experimental data.

Keywords: Mars Science Laboratory, Heatshield, Coating, NuSil, Equilibrium chemistry, Ablation, Pyrolysis.

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Effect of out-gassing on the onset of transition in hypersonic boundary layers

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Abstract

In the high-speed/high-enthalpy environment of entry into a planetary atmosphere, boundary layer transition (BLT) plays a key role on aerothermal heating. In such an environment, BLT is coupled with other physical phenomena such as the ablation of the Thermal Protection System (TPS) [1]. Ablative heatshields are designed to alleviate the high heat flux at the surface through pyrolysis of their polymeric matrix and subsequent fiber ablation [2]. Understanding the interaction between material thermal response and flow instability is crucial in designing an affordable and effective TPS. Ablation impacts BLT through three main avenues: gas injecting into the boundary layer from the wall, changing the surface heat transfer due to wall-flow chemical reactions, and modifying surface roughness via ablative processes [3]. In the present work, we examine the effect of out-gassing associated with surface pyrolysis on the onset of laminar-turbulent transition. Employing the concept of intermittency [4], we create a map corresponding to the surface pressure as a measure of the probability that at a given point in space and time the flow is turbulent. To develop correlations for transition induced by the ablation product boundary layer interaction, we start with the simplest form of a smooth but blowing surface. Although the blowing rate is not uniformly constant across the wetted face of the heatshield, as a first approximation, we assume that the gas constantly blown into the boundary layer is only present where maximum wall heat flux has been observed and is associated with higher intermittency in the transition map. The surface is assumed to be in radiative equilibrium, fully catalytic to ions but supports only homogeneous surface reactions. To model the effect of ablation-induced out-gassing on transition onset, we compare non-injecting gas boundary layer as a baseline case with the cases with various blowing rates. Injecting gas is applied to the regions of the wetted surface where transition has been observed previously. Those regions are identified by a map intermittency distribution on the heatshield. To identify the role of mass addition on the boundary layer transition, knowledge of the blowing gas composition matters. In that regard, we first inject the same gas as that of the freestream gas and compare the results against the case of injecting some inert species that has comparable molecular weight such as CO representing ablation products. Through a parametric study, we investigate the various levels of blowing rate to determine how the onset of transition is altered. The results suggest that strong out-gassing promotes shifting the onset of transition in the windward of the wetted surface of the heatshield while reducing the wall heating augmentation Fig. 1.

Keywords: laminar-turbulent transition, hypersonic boundary layers, out-gassing-induced transition

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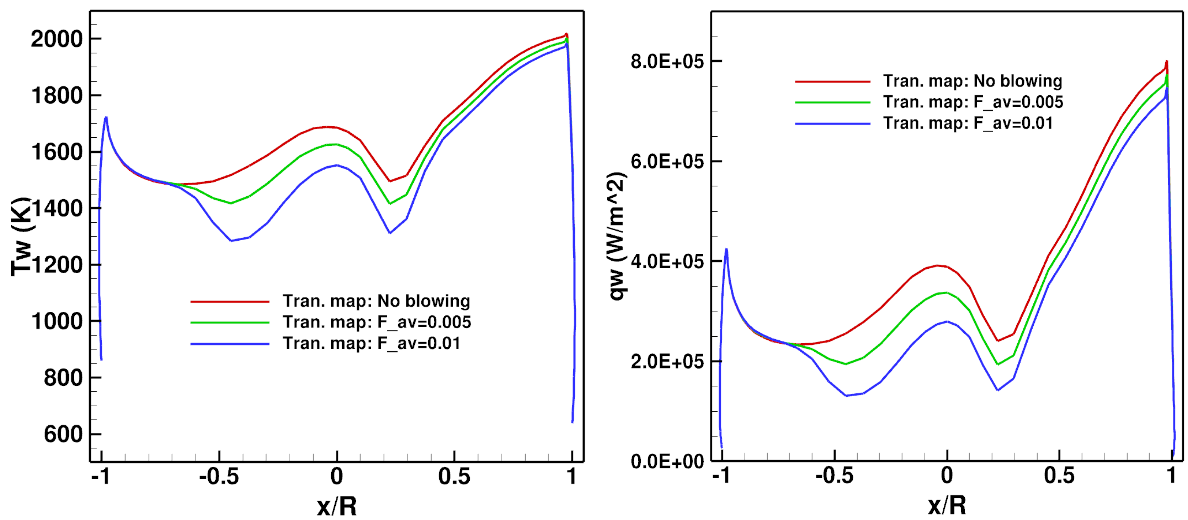

Figure 1: Comparison of predicted centerline (a) wall temperature and (b) heat flux using transition map model with the different non-dimensional blowing rates of $F_{avg} = (\rho u)_w/(\rho u)_\infty$ which is the ratio of the momentum at the wall to the one in freestream for the Mars Science Lab heat shield forebody geometry. Centerline coordinate is normalized by the heat shield radius.

DETERMINATION AND COMPARISON OF THE CHARACTERISTICS OF NEW CLASS OF ABLATIVE MATERIALS

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ABSTRACT

Ablative materials are used for various applications, such as solid rocket motors, missile launching systems, and thermal protection systems (TPS) for re-entry vehicles in the defense and aerospace industries. High-performance aerospace systems require innovative ablative material systems to meet their stringent requirements. In order to determine characteristics of these new ablative materials, various material response (MR) codes were developed and used. One of these MR codes, MESA (Material Erosion and Stress Analysis Code) developed at Pennsylvania State University by F.B. Cheung and B.C. Yang in order to determine the ablation properties for a class of glass/phenolic ablatives. MESA code has the capability to predict mechanical erosion due to particle impact, thermochemical ablation due to imposed heat flux, thermal buckling due to internal pore pressure, and thermal characteristics 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 computations were conducted using the MESA code to predict the performance of ablatives, such as H41N (glass/phenolic) and MXBE-350 (rubber modified glass/phenolic) and compared with the experimental data performed at FMC Corporation Naval Systems Division by Cheung and Yang [1, 2]. As a result, the MESA code was validated by comparing the numerical results with experimental data.

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^{o}C) are provided by J. B. Henderson [3].

For the purpose of using this MR code, validation of the code is performed by using a known ablative material called MXBE-350. Exposition of hot gases to this ablative material is lasted approximately 5.2 seconds. The results obtained using this code and the study performed by Cheung and Yang [2] are compared in terms of thermochemical ablation, mechanical ablation, and instantaneous surface location. After this validation of usage of the MR code, characteristics of the

new ablative materials will be studied by using this code. Comparison of the various material properties and the effects of these properties on ablation will be investigated.

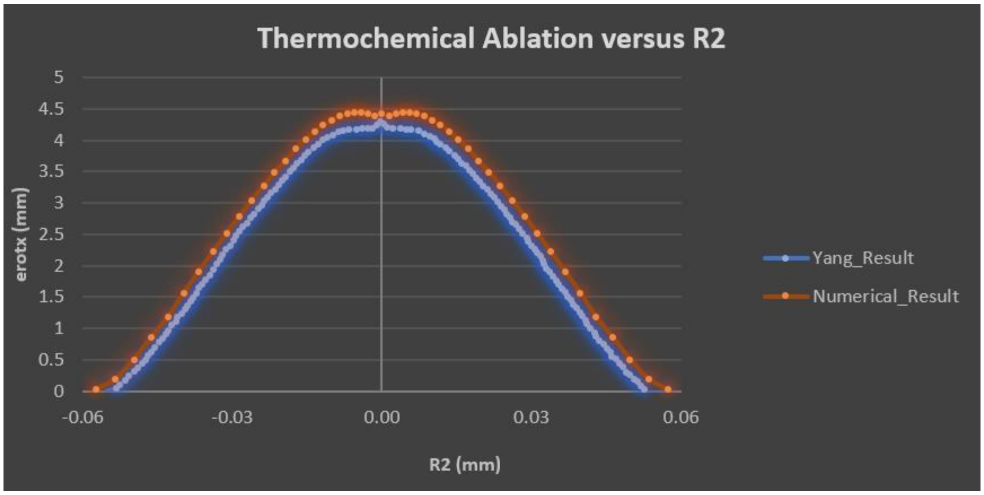

Figure 1. Thermochemical ablation versus radius of the ablative material.

In Figure 1, comparison of the thermochemical ablation obtained by Cheung and Yang's study and the current MR model using the MESA code is shown. The maximum difference between the two comparison is about 3%.

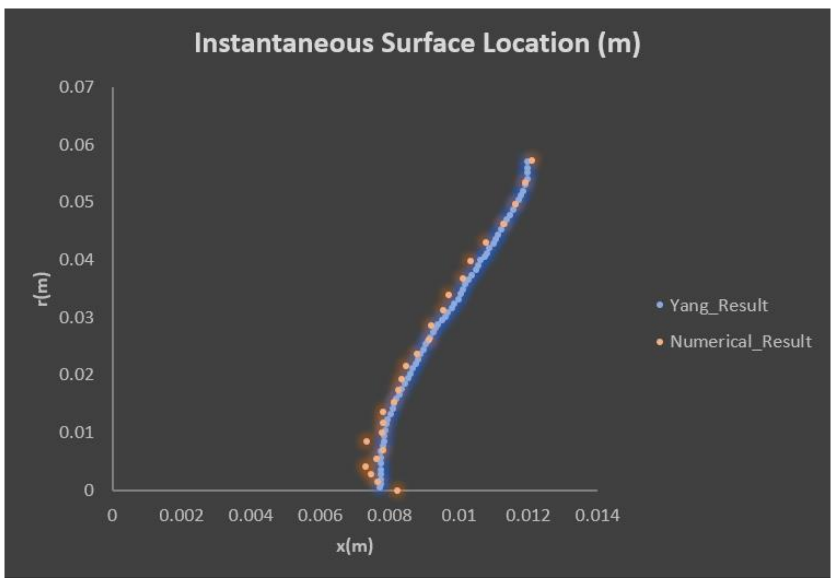

Figure 2. Instantaneous surface location (m).

In Figure 2, the instantaneous surface location depends on time of ablative material is shown. At the end of the regression process, there are differences between the results. The discrepancy of the studies will be investigated. In Figure 3, mechanical ablation result is seen for 5.2 s of exposure time. There are also some minor differences between these two sets of results.

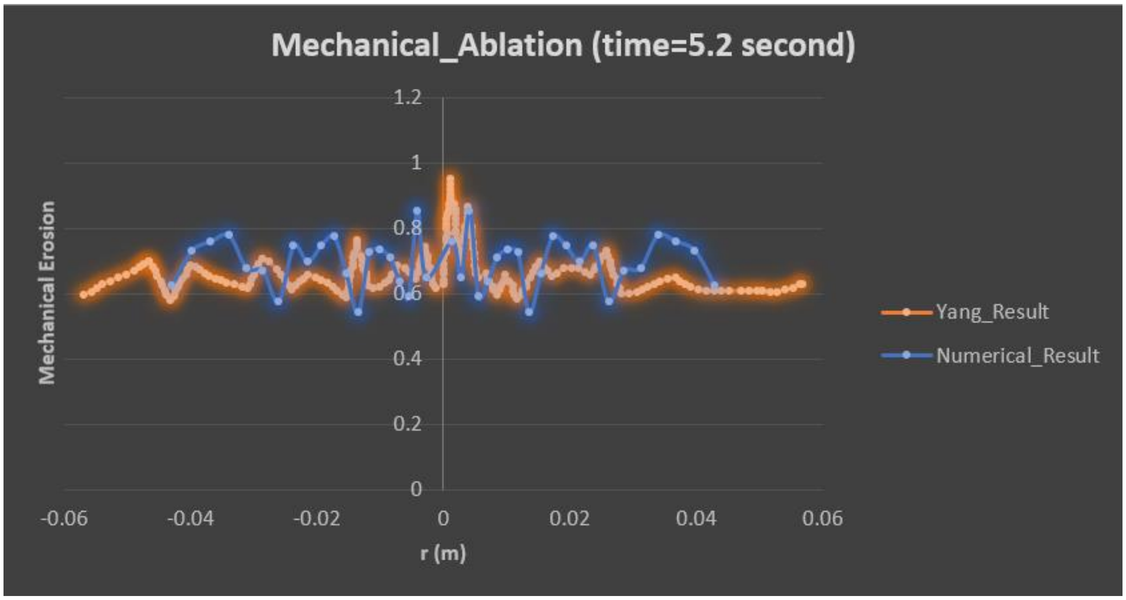

Figure 3. Mechanical ablation versus radius of the ablative material.

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Microstructure investigation of elastomeric TPS char based on solid rocket motor experiments

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ABSTRACT

Thermal protection systems (TPS) research has a significant part in the development of Rafael's products for aerospace applications, such as internal insulation for solid rocket motors (SRM) and nozzles. Oxyacetylene facilities and sub-scale motors are used to simulate high temperature environment experienced inside a rocket motor chamber and to screen candidates of TPS materials. The results are compared to full-scale firing of SRM (Figures 1-2).
In the present research, we will demonstrate the contribution of attack angle of gases on pore structure diversity of elastomer-based charred material – using Micro x-ray tomography. The density, porosity and thermal conductivity (Figure 3) of the charred TPS will be discussed, as well. Using XRD, the evidence of high density char is investigated in attempts to find the root cause (coking phenomena, carbon-silica reactions). Ablation sensors are fabricated and tested for the temperature evolution near the surface of the TPS, showing irregular temperature behavior due to the blowing effect (Figure 4).

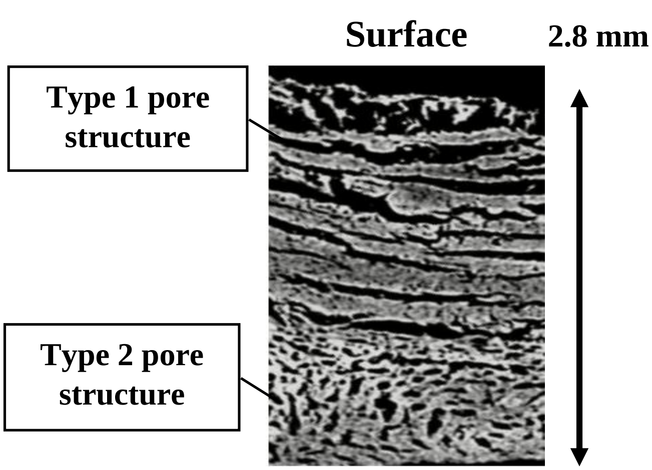

Figure 1: Charred TPS of full-scale motor firing

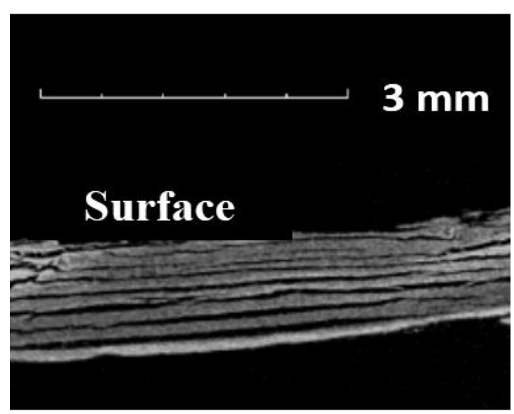

Figure 2: Charred TPS of sub-scale motor firing

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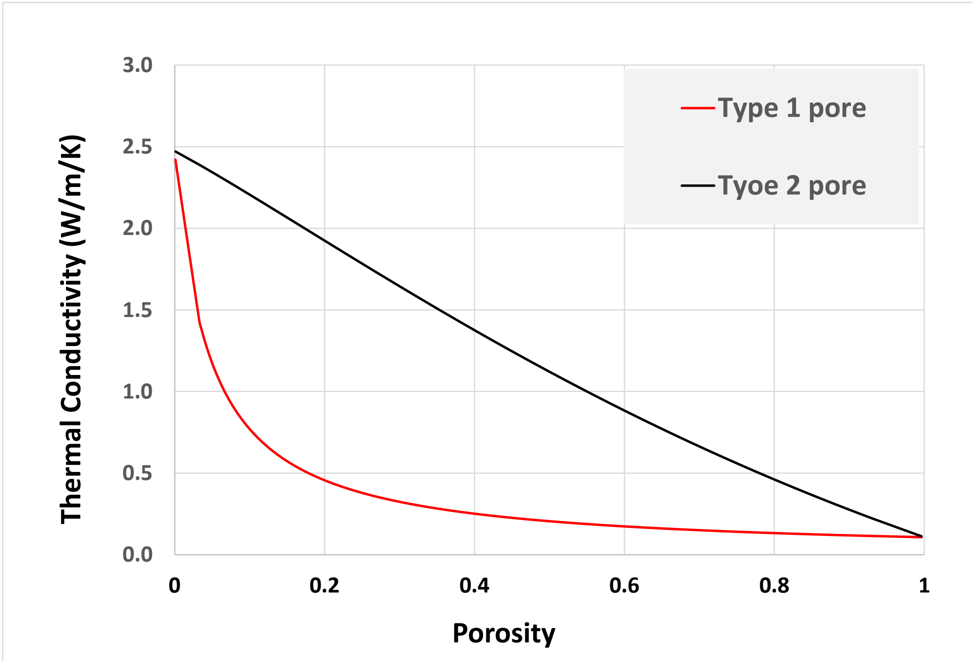

Figure 3: Predicted Thermal conductivity vs. pore microstructure

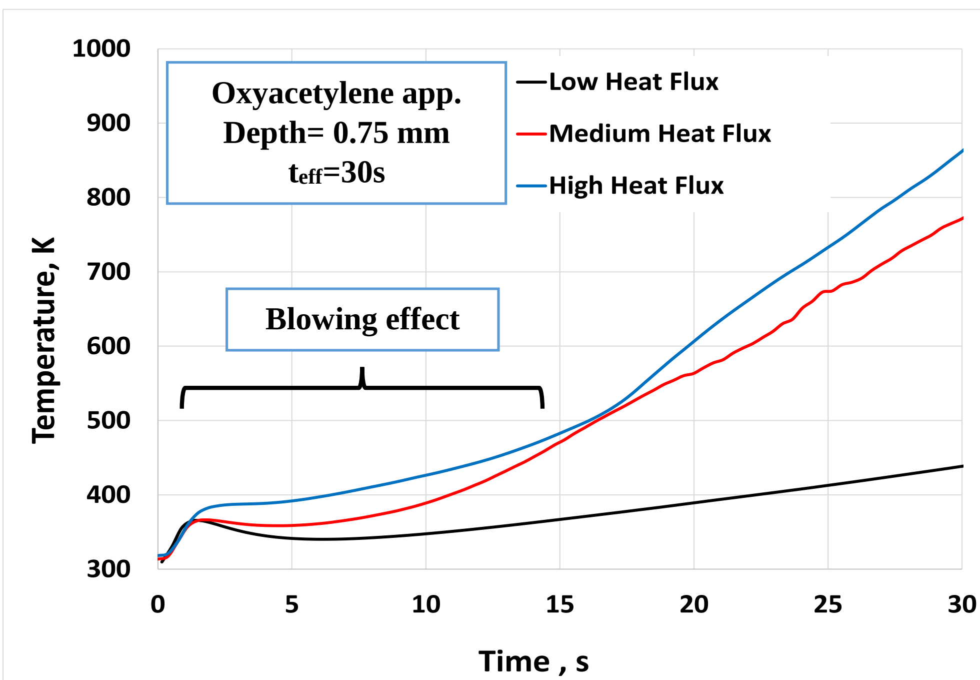

Figure 4: Temperature evolution inside ablation sensor of elastomeric TPS

Model and Characterization of Ablative Composite Material Based on Cork and Silicone Rubber

Noa Eizckoviz

Abstract

A missile executing hypersonic flight through a planetary atmosphere is exposed to severe heating. This heating, caused mainly by stagnation of the flow and by the extreme viscous dissipation that occurs within hypersonic boundary layers, is liable to damage the missile unless it is protected by suitable (robust) thermal insulation. In this work a critical evaluation of the performance of the new cork/silicone composite is presented. First, a model of the heating and ablation of an insulated missile surface, and its simplification, is discussed. Next, the experimental determination of necessary thermophysical properties is presented and critically evaluated. Following this, calibration and verification of the modeling approach is demonstrated by comparing results from computational analyses of heating and ablation under high and low pressure conditions, to those achieved in relevant arc-plasma wind tunnel experiments. Finally, the computational approach is used to predict the performance of the new insulation material during realistic missile flight trajectories.

Keywords: Heat Transfer, Mass Transfer, Ablation, Thermal Insulation

HyCUBE: A reconfigurable cubesat-like platform for hypersonic flight testing

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Abstract

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Arc jet testing and evaluation of Mo–Si–B coated Mo and SiC–ZrB_2 ceramics

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The transition from blunt leading edges to sharp leading edges on re-entry aircrafts is necessary to increase both maneuverability and safety. However, the oxidation resistance of current materials is inadequate for the extreme conditions experienced by sharp leading-edge re-entry vehicles. The Mo–Si–B alloy system has been utilized to design a multilayer coating that has the ability to protect from 800 to 1700 ◦C. Substrates of Mo and ZrB_2–50 vol% SiC with a flat profile were coated with the Mo–Si–B based coating and evaluated using arc jet testing performed at NASA Langley Research Center. Heat fluxes of 2.5 to nearly 3.5 MW/m^2 and surface temperatures of 1500–1650 ◦C were achieved during the 20-min tests. The samples presented in this study showed <3% mass loss and retention of sample shape and integrity, demonstrating the robust environmental protection under a simulated hypersonic environment offered by the Mo–Si–B based coating on refractory metals and ceramics.

PROBABILISTIC RISK ANALYSIS AND MARGIN PROCESS FOR A FLEXIBLE THERMAL PROTECTION SYSTEM

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Abstract: The Low Earth Orbit Flight Test of a Inflatable Decelerator (LOFTID) Reentry Vehicle's Flexible Thermal Protection System (FTPS) protects the aeroshell inflatable structure (IS) from over-heating during atmospheric entry. For a given FTPS size and entry trajectory, critical FTPS and IS temperatures must be predicted in order to prescribe design modifications to the FTPS and determine a corresponding allowable entry heat load range.

There is uncertainty in the critical temperature predictions due to the uncertainties that exist in atmospheric entry aeroheating environments and the thermal response of the FTPS/IS materials. These uncertainties are mitigated by tailoring the planned entry heat load and FTPS thickness in order to apply margin and safety deltas to the FTPS/IS critical temperature predictions. Entry vehicle heat shields are traditionally conservatively over-sized for the heat loads that are experienced along the entry trajectory by designing to survive stacked worst-case scenarios. Additionally, the conventional heat-shield design and margin process offers very little insight into the risk of over-temperature during flight and the corresponding reliability of the heat shield performance [1,3].

Since the LOFTID project is an experimental flight, it is desired to drive the FTPS and IS in the entry environment to temperatures that cover a large range of their thermal response models' applicability. This will allow the thermal response models to be better improved and validated post-flight using LOFTID's extensive instrumentation embedded within the aeroshell.

A probabilistic margin process can be used to calculate the amount of margin that is necessary and the corresponding allowable heat load for an entry vehicle to survive at a specified level of reliability while allowing the aeroshell to be pushed to adequately high temperatures in flight [2,3,4]. It does so by rigorous calculation of the risk of the critical temperature exceeding their limits. The initial entry state (entry velocity, flight path angle, and entry mass) determines the expected atmospheric entry conditions and resulting heat load that the vehicle will experience. Since there is some flexibility in LOFTID's initial entry state this process can be used to select an appropriate combination of entry state parameters and FTPS size that allows the aeroshell to survive entry with the desired level of reliability. This probabilistic margin process allows engineers to make informed aeroshell design, entry-trajectory design, and risk trades while preventing excessive margin from being applied.

The probabilistic margin process is carried out by an uncertainty analysis method which employs an end-to-end Monte Carlo simulation. Three Monte Carlo simulations are run to complete the end-to-end process. The end-to-end Monte Carlo simulation propagates the uncertainties in the trajectory and aeroheating model into the FTPS and RV thermal models to quantify the resulting uncertainty of the FTPS/IS thermal response.

Summary of Results: Using the end-to-end Monte Carlo process, the risk of aeroshell over-temperature and the reliability of successful FTPS performance was calculated. Quantified modifications to the atmospheric entry heat load and mitigation to conservatism in the FTPS/IS thermal response models were recommended to reach a more acceptable calculated risk level. The entry heat load can be modified by changing the entry velocity, flight path angle, or entry mass of the entry vehicle.

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Table-Top Shock Tunnel for Studying Thermochemical Nonequilibrium Chemistry in Hypersonic Flows

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Abstract

Hypersonic flight through an atmosphere generates a thin, high-temperature, shock layer that surrounds the vehicle surface, typically a heat-shield material. The gas in the shock layer is far from equilibrium and may contain atmospheric species in a dissociated state as well as ablation products from the heat shield. Current models are empirical and are unable to predict conditions in a hypersonic shock layer, and new models under development are limited by the paucity of high-quality data needed for their refinement and validation. The table-top shock tunnel (TTST) under construction will embody a new experimental approach for measuring shock layer chemistry under relevant hypersonic conditions. The TTST consists of a custom vacuum system, including a hypersonic pulsed molecular beam, a main test chamber, a Schlieren system for optical imaging of a shock layer, and a differentially-pumped mass spectrometer detector to characterize the hypersonic beam. The pulsed molecular beam, when targeted at a small blunt object in the test chamber, can generate a shock layer that mimics the shock layer formed in front of a hypersonic vehicle, in an instrument that is a mere 2 m long. Unlike large shock tunnel facilities, the beam, and therefore the shock layer, can be generated at 2-5 times per second for hours or even days with repeatable conditions. Such test frequency and repeatability should enable existing optical diagnostic techniques to measure thermochemical quantities with unprecedented accuracy and precision at a fraction of the cost compared to existing shock tunnel facilities. The synergistic combination of computational modeling and unprecedented experimental data should lead to a fundamental understanding of shock layer chemistry and physics that goes far beyond current knowledge. The ultimate practical outcome of the near- and long-term research enabled by this new instrument will be accurate predictive models of nonequilibrium hypersonic flows.

A melting-ablation model for arc-jet electrodes

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Abstract

Electrodes erosion is one of the main concerns for the operation of high-power arc-jet facilities. Copper cathodes and anodes, subject to strong electric current arcs, reach temperatures high enough to trigger melting and evaporation of the material. In turn, this limits the operating time of the components, as well as inducing chemical pollution in the flow due to the erosion products. Here we present a one-dimensional numerical model to study the electrodes ablation. The latter solves the Stefan problem in a one-dimensional slab to determine the time evolution of the melt front. The evaporation of the molten material is estimated by the Knudsen-Langmuir law, based on the material saturated vapor pressure. Surface recession is then computed from the evaporation mass flux and material density.
Future work includes the coupling of the material response code to a 1D flow solver, to implement a more precise model for surface energy and mass balance, as well as the extension of the solver to treat multidimensional problems.

Keywords: Arc-jet electrodes, Melting, Evaporation

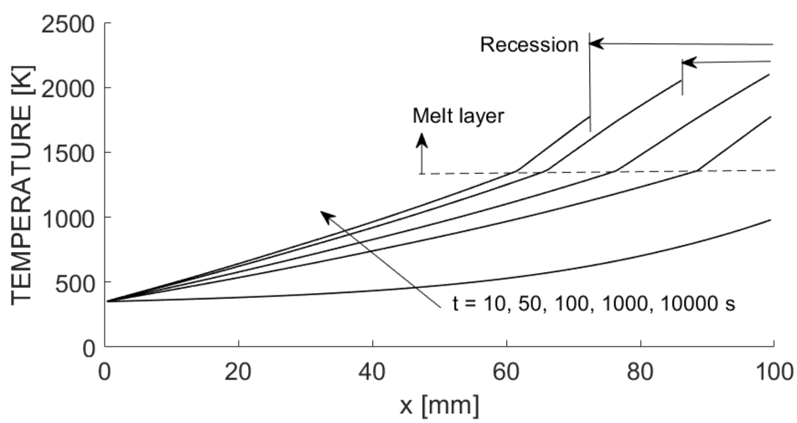

Figure 1: Test case showing the melting-ablation of a 100 mm copper slab, with an imposed heat flux of 7 MW/m² *on the right edge and a constant temperature of 350* K *on the left edge. The model is able to track the evolution of the melt front and to compute the recession on the surface due to evaporation.*

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Analysis of Spallation Particles Using Arc-Jet Experiments

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Abstract

Experiments were conducted using a hypersonic arc-jet facility to investigate the spallation of solid particles ejected off of thermal protection system material. To assess the impact of surface shear and oxidation on the rate of spallation, samples with different geometries were exposed to different high enthalpy environments to produce the same nominal heat flux. Particles ejected from the sample were quantified and tracked using particle tracking velocimetery.

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