9th Ablation Workshop

August 30 - September 1 2017
Montana State University
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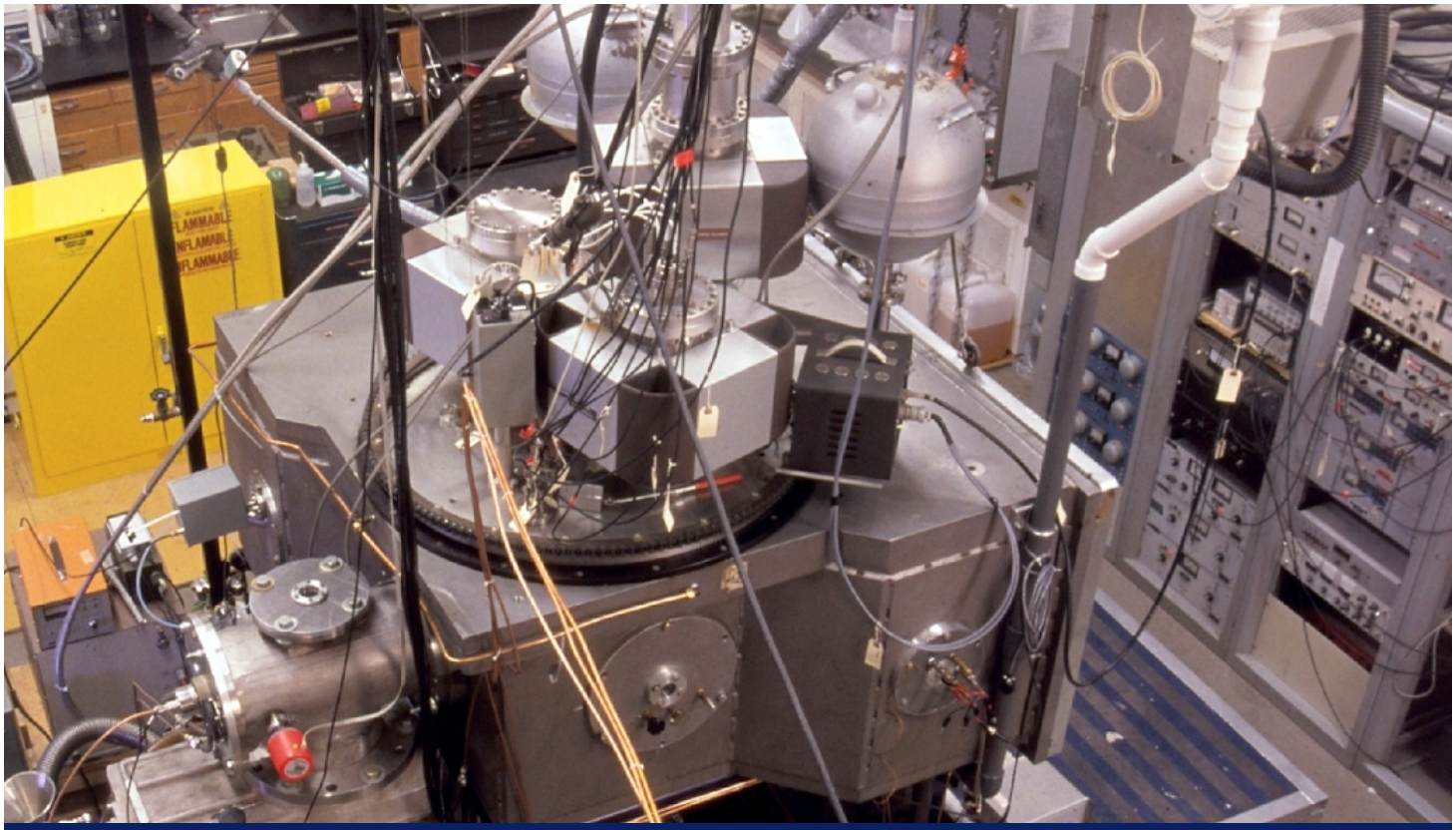

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Abstracts of the 9th Ablation Workshop

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Abstracts of the 9th Ablation Workshop
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CONFERENCE PROGRAM

Day 1: August 30, 2017

Introduction and Keynote Lectures

Chair: Alexandre Martin, University of Kentucky, USA

Modeling Material Response at the Macro Scale – I

Chair: Michael Wright, NASA Ames Research Center, USA

Multi-Scale Modeling – I

Chair: Kelly Stephani, University of Illinois, USA

Oxidation of Carbon

Chair: Thomas Schwartzentruber, University of Minnesota, USA

Day 2: August 31, 2017

Emerging Materials and Methods

Chair: Charles Bersbach, Raytheon Missile Systems, USA

Modeling Material Response at the Macro Scale – II

Chair: Mark Ewing, Orbital ATK, USA

Multi-Scale Modeling – II

Chair: Nagi Mansour, NASA Ames Research Center, USA

High-Enthalpy Experiments

Chair: Erica Corral, University of Arizona, USA

Day 3: September 1, 2017

ITAR Session – Restricted Access

Chair: Stan Bouslog, NASA Johnson Space Center, USA

Posters

Current Technology Investments in the Entry Systems Modeling Project

Michael J. Wright[a,*]

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Overview of AFOSR Interests in Ablation

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Development of the European Conformal Ablative-Charring material and performances assessment

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Abstract

The state of the art thermal protection material for high speed Earth Return Capsule is undoubtedly light weight ablator based on carbon fiber impregnated by phenolic resin. The most famous example is the PICA material (Phenolic impregnated Carbon Ablator) that flew on the faster man-built Stardust Capsule. In Europe, such material development started in 2004 with ASTERM family. The standard ASTERM version is using a highly porous rigid substrate impregnated with phenolic polymer. The composite proved to be well suited for 1 m scale probe where monolithic heat- shield could be directly milled from rough cylindrical preform. For larger vehicle, heat-shield must be assembled from multiple pieces or tiles since the material shows a brittle behavior and low strain to failure.
Since few years, Airbus Safran Launchers has on going activities to extend the ASTERM material family and to mature technology on conformal charring ablator with the goal to tackle this standard version thermo-mechanical limitation. Instead of rigid felt, this new material uses a flexible carbon preform that could be easily shape by molding process. After curing, it results in a rigid ablator with potential curved surface. Due to the properties of the felt, C-ASTERM will reveal better compliance behavior with regard to the sub-structure compared to the standard rigid ASTERM.
In the framework of DECA (Development of European Conformal Ablator) ESA's TRP, a conformal ablator material will be manufactured and deeply characterized.
The proposed test plan not only includes laboratory thermo-physical and thermo-mechanical characterization (mainly performed in Tecnalia lab.) but also arc jet plasma campaign both in Airbus Safran Launchers (wedge configuration) and DLR (stagnation point configuration) facilities. This unique plasma test was also the opportunity to qualify advanced measurement sensors for the ablation characterization.
A numerical thermal and ablative model of the C-ASTERM material is built by a mix of elementary characterizations and plasma results cross checking. The model is mathematically closed by a set of assumptions and laws (when missing) taken from the standard ASTERM material.
Finally, a 1 m scale tiled static demonstrator made of standard and conformal ASTERM will be bonded on a representative CFRP-composite honeycomb sandwich structure to validate bonding and assembling process previously adjusted in laboratory and reach a TRL of 4.

Keywords: Conformal ablator, thermomechanical model

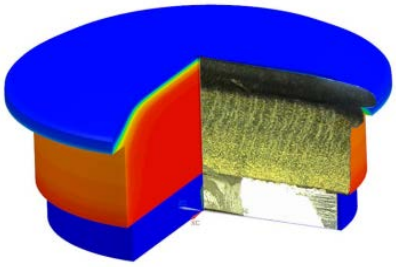

Figure 1: *In-depth density profile on a stagnation point configuration*

Figure 2: *1 meter diameter demonstrator in Standard (dome) and Conformal (tile) Asterm*

Thermal Protection for Mars Sample Return Earth Entry Vehicle: A Grand Challenge for Design Methodology and Reliability Verification

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Mars Sample Return is our Grand Challenge for the next decade. Human missions to Mars (and return) remain the centerpiece of NASA's long-term exploration strategy for the next 20-30 years. Mars sample return missions will happen before humans set foot on Mars. We should anticipate that the first MSR mission will take place before 2030. The TPS community should plan now to deliver essential new design and verification capability to enable this mission.

TPS nominal performance is not the key challenge. Several successful missions have been flown to more severe environments. The main difficulty for designers is the need to verify unprecedented reliability for the entry system: current guidelines for prevention of backward contamination require that the probability of spores larger than 1 micron diameter escaping into the Earth environment be lower than 1/million for the entire system, and the allocation to TPS would be more stringent than that. For reference, the reliability allocation for Orion TPS is closer to 1/1000, and the demonstrated reliability for previous human Earth return systems was closer to 1/100. Improving reliability by more than 3 orders of magnitude is a grand challenge indeed.

Historically, TPS and primary structures have been exempted from fault-tolerance requirements that are levied on other subsystems, because the mass penalty for redundancy can be severe. Nevertheless, structural design often includes elements that support secondary load paths when structure is damaged locally. Similar concepts should be explored for TPS, too, to deliver graceful degradation of performance if local damage is experienced. Conley and Kminek [Ref. 1] have noted that the reliability requirements for MSR demand a new approach overall campaign and design: *"Risk-based design, accounting also for common cause/mode failures, drives redundancy and diversity of system design... Fault tree needs to become the best friend of systems engineers from the very beginning."* Can we break free of the assumption that a passive single-string design is optimal, and explore alternatives that appear more complex but reduce the reliability verification burden for any individual element?

The TPS community must embrace the possibility of new architectures that are focused on reliability above thermal performance and mass efficiency. MSR EEV will be hit with MMOD prior to reentry. A chuteless aeroshell design which allows for self-righting shape was baselined in prior MSR studies, with the assumption that a passive system will maximize EEV robustness. Hence the aeroshell along with the TPS has to take ground impact and not break apart. System verification will require testing to establish ablative performance and thermal failure but also testing of damage from MMOD, and structural performance at ground impact. Mission requirements will demand analysis, testing and verification that are focused on establishing reliability of the design. Design should avoid features that lead to failure across the entire mission operation, when possible. But design should also consider interventions that mitigate the consequence of off-nominal states that might be detected.

Ablative TPS for Mars Sample Return was explored during the (1997 – 2005) joint effort by NASA and CNES. That effort led to baselining Carbon-Phenolic and SLA for heat-shield and backshell respectively, primarily because they had the most flight heritage of any available material systems. Since then, however, we have had challenges with both Carbon Phenolic and SLA. The heat-shield for extreme entry environment technology (HEEET) system has been developed in response to the raw material supply issues for heritage carbon phenolic (lack of similar precursor rayon) and atrophy of the manufacturing base for processing chop molded carbon phenolic. Given the difficulties that were recently experienced in reconstituting Avcoat for Orion, there is considerable risk that performance of newly-manufactured Carbon Phenolic will differ from heritage capability, and subtle differences may not be exposed in ground testing of small components. SLA-561 V went through its own distinct challenges when failure was observed in ground test at around 100 W/cm2, in high shear conditions. This failure demonstrated

sensitivity to environment changes that were expected to be benign, but exposed an unanticipated mode of material loss.

The lack of broad operational experience for any candidate TPS means that there is no strong statistical evidence of reliability across a comprehensive range of possible environments. Hence, acceptable reliability will require understanding the causes that lead to failure and designing to avoid them if possible or margin against them with confidence will be required for MSR EEV. Physical models will need to represent failure precursor behavior in each material and at material interfaces in the integrated system. These models will need to capture failure onset in ground tests at a range of operating conditions, to build confidence that they accurately predict material response behavior at mission operating conditions. Furthermore, models will need to include all plausible off-nominal states of the heatshield, due to degradation from all loads endured prior to the entry phase of the mission. The demand for modeling detailed thermostructural response is unprecedented, and represents a huge opportunity for nascent efforts in computational design of materials.

In this proposed talk, we will first describe and illustrate, through examples, how advances in 3-D weaving allowed us to find solutions to challenging TPS problems. The second part of the talk will focus on the grand challenge of MSR EEV TPS and the need for innovative approaches to address challenges in modeling, testing, manufacturing and verification.

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Full-scale Mars Science Laboratory Tiled Heatshield Material Response

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Abstract

During Mars atmospheric entry, the Mars Science Laboratory (MSL) was protected by a 4.5 meters diameter ablative heatshield assembled in 113 tiles [1]. The heatshield was made of NASA's flagship ablative material, the Phenolic Impregnated Carbon Ablator (PICA). The objective of this work is to analyze the effects of tiling on the material response of the full-scale MSL tiled heatshield. The traditional assumption of one-dimensional simulation for material response will be verified at different locations of the heatshield. The Porous material Analysis Toolbox based on OpenFOAM (PATO) [2, 3] is used for this study. The governing equations are volume-averaged forms of solid mass, gas mass, gas momentum and total energy conservation, including pyrolysis gas production. The thermodynamics and chemistry properties are computed using the Mutation++ library [4]. The boundary conditions at the heatshield front surface are interpolated in time and space from the aerothermal environment [5] generated with the Data Parallel Line Relaxation (DPLR) code [6] at discrete points of the MSL trajectory. The two million cells mesh created in Pointwise and the velocity inside the material in the shoulder region are represented in Figure 1 and 2, respectively. Three-dimensional effects are pronounced at the heatshield shoulder where maximum heating occurs. The present work highlights a capability of PATO ; it constitutes the first demonstration of a three-dimensional material response simulation of a full-scale ablative heatshield with tiled interfaces.

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

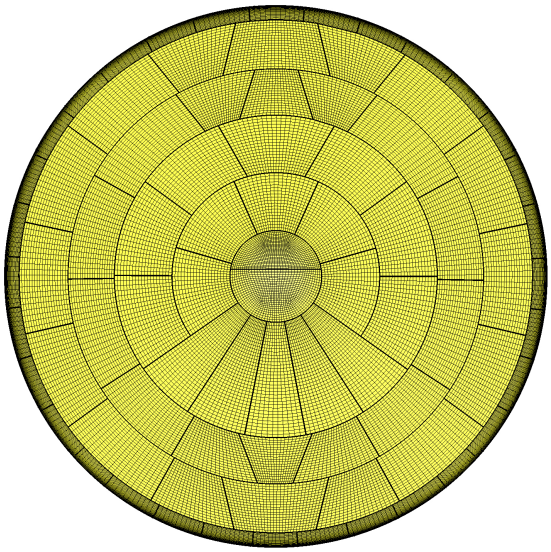

Figure 1: MSL tiled heatshield mesh.

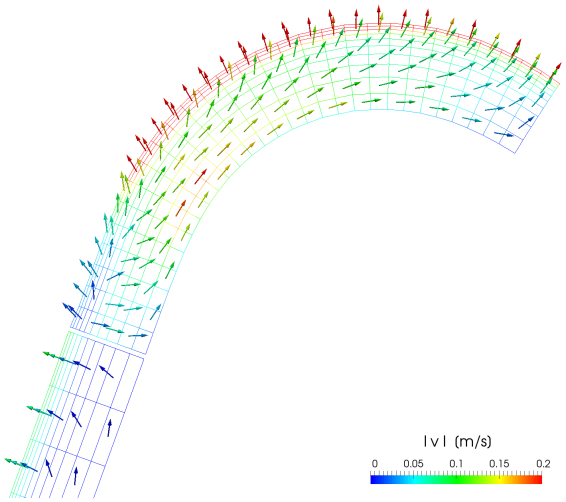

Figure 2: Velocity field at a cross-section of the leeside heatshield shoulder.

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Overview of the Icarus Material Response Solver

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[c]*Department of Mechanical Engineering, University of Kentucky, Lexington, KY 40506, USA*

Abstract

An overview, and current development status of the Icarus material response solver is presented. Icarus [1] is a three-dimensional, unstructured, finite volume material response solver under active development at NASA Ames research center, and is intended to enable multi-dimensional ablator response simulations on complex geometries.

This presentation will provide an overview of the physical models available in the current implementation, as well as the modular code structure, which enables straightforward extensibility to accommodate new models, as they become available from complementary research efforts. Recent verification and validation studies will be presented, as well as selected application cases. Additional detail will be provided for the approach to mesh motion that is used, as this is aspect is often often adversely affects the robustness of 3D solvers. Icarus employs the radial basis function (RBF) method[2], which is particularly well suited to problems with unstructured grids and surface driven motion. Verification and timing studies for the current RBF implementation in Icarus will be presented.

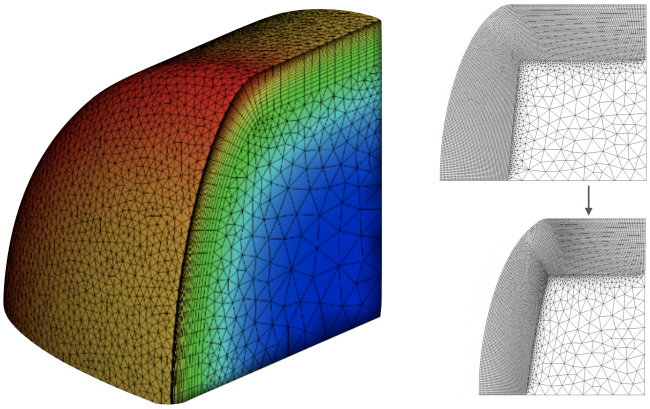

Figure 1: Demonstration simulation of an Iso-Q arc jet article using a hybrid unstructured mesh(*left*), and illustration of the radial basis function mesh motion applied to an ablating Iso-Q(*right*).

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Unified flow-material simulations of light-weight carbon ablators in the VKI Plasmatron: a step forward

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Abstract

Carbon-based porous ablators are used to protect spacecraft during the atmospheric entry phase of interplanetary missions. Advances in modeling the interaction between a chemically reactive boundary layer and the spacecraft heat shield can bring substantial benefits to the overall mission mass budget.

During the last years, a unified approach, which uses a strongly coupled modelization of the flow and the porous material, has been implemented within the multi-dimensional tool Argo developed at Cenaero. The methodology is based on the volume averaging theory applied to the reactive Navier-Stokes equations. This continuum description is flexible enough that it can go smoothly from a plain fluid region to a receding porous medium. The material porosity is itself a variable smoothed on the grid during initialization and then computed to track the evolution of the reactive porous medium. In the present activity we use the developed tool to simulate the experiments carried out in the high-enthalpy Plasmatron facility at the von Karman Institute (VKI) on a carbon-fiber preform. A full Plasmatron experiment is simulated (Fig. 1) and the transient numerical results are compared with the optical measurements performed during the experimental test.

Recent developments of the tool include the possibility of simulating the thermal decomposition of the phenolic resin of charring light-weight ablators. The pyrolyzing polymer is assumed to decompose through a number of pyrolysis reactions, each characteristic of a fictitious solid species composing the resin, and the rate of decomposition of each resin compound is expressed by means of an Arrhenius-type law. Difficulties encountered and solutions applied during the development of this "pyrolysis module" are thoroughly reviewed, and preliminary results are presented.

Finally, updates on the development of the gas-surface interaction (GSI) module of the VKI Mutation++ library are presented. The library has been conceived to be easily integrated within any CFD solver and it currently solves the mass and energy balances at the gas-surface interface featuring several GSI mechanisms for both catalysis and ablation. Argo already makes use of the Mutation++ library for the evaluation of thermodynamic and transport properties of the high-enthalpy flows, as well as for the computation of the chemical source terms in the gas phase. Ideally, in the future, it will make use of the GSI features of Mutation++ as well. This further step will allow the integration of newly developed, and more complex, GSI reaction mechanism with limited effort.

Keywords: Porous Ablators, Volume-Averaged Navier-Stokes equations, Pyrolysis, Gas-Surface Interaction Modeling

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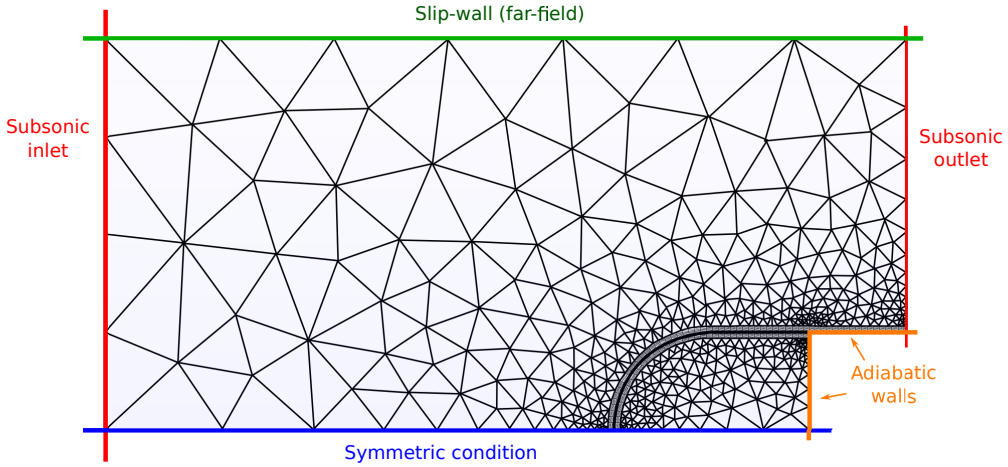
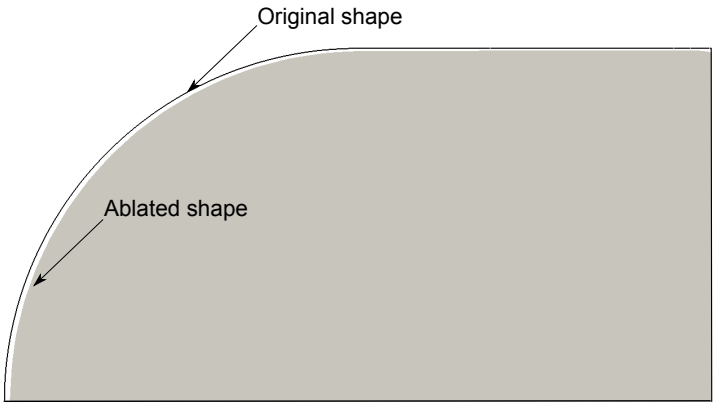


(a)



(b)

Figure 1: (a) Computational domain with boundary conditions for the Plasmatron experiment; (b) shape change of the ablated carbon-preform sample.

An introduction to the derivation of surface balance equations without the excruciating pain

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Abstract

Analyzing complex fluid flow problems that involve multiple coupled domains, each with their respective set of governing equations, is not a trivial undertaking. Even more complicated is the elaborate and tedious task of specifying the interface and boundary conditions between various domains. This paper provides an elegant, straightforward and universal method that considers the nature of those shared boundaries and derives the appropriate conditions at the interface, irrespective of the governing equations being solved. As a first example, three well-known interface condition are derived. Finally, the set of boundary conditions necessary to solve a baseline aerothermodynamics coupled plain/porous flow problem is derived, and the following surface balance equations are obtained:

$$\boxed{\left[\dot{m}'' Y_i - \rho_g D \frac{\partial Y_i}{\partial x}\right]_f = \left[\dot{m}'' Y_i - \rho_g D \frac{\partial Y_i}{\partial x}\right]_p} \tag{1}$$

$$\boxed{\left[\rho_g u^2 + p - \tau_{xx}\right]_f = \left[\phi\rho_g u^2 + p - \alpha_s \phi\mu \frac{2u}{\sqrt{K_{xx}}}\right]_p} \tag{2a}$$

$$\boxed{\left[\rho_g uv - \tau_{yx}\right]_f = \left[\phi\rho_g vu - \alpha_s \phi\mu \left(\frac{v}{\sqrt{K_{xx}}} + \frac{u}{\sqrt{K_{yy}}}\right)\right]_p} \tag{2b}$$

$$\boxed{\left[\rho_g uw - \tau_{zx}\right]_f = \left[\phi\rho_g wu - \alpha_s \phi\mu \left(\frac{w}{\sqrt{K_{xx}}} + \frac{u}{\sqrt{K_{zz}}}\right)\right]_p} \tag{2c}$$

$$\boxed{\left[\rho_g uh - (\tau_{xx}u + \tau_{xy}v + \tau_{xz}w) + \dot{q}_x'' + \sum J_{x,i} h_i\right]_f = \left[\phi\rho_g uh - \alpha_s \phi \frac{\mu}{\sqrt{K_{xx}}}\left(u^2 + v^2 + w^2\right) + \dot{q}_x'' + \sum J_{x,i} h_i\right]_p} \tag{3}$$

For instance, by simplifying this last equation using the total conservation of mass and neglecting the work performed by shear on both sides of the surface reduces this equation to Eq. (6) of Milos and Rasky[1]:

$$\left[-k_T \frac{\partial T_T}{\partial x} - k_v \frac{\partial T_v}{\partial x} - \sum_i \rho_g h_i D \frac{\partial Y_i}{\partial x}\right]_f = \dot{q}_x'' + \dot{m}''(h_p - h_f) \tag{4}$$

Keywords: Surface balance, Ablation , Thermal protection system, Porous media

References

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Analysis of Ablative TPS Using Scale-Bridging Molecular Dynamics

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Abstract

Pyrolysis of a phenolic resin polymer is a well-known heat removal mechanism in charring ablators, but the process has not been well-quantified. Here we study the ablation of polymer-based thermal protection systems (TPS) using scale-bridging simulations. A crosslinked phenolic formaldehyde resin is modeled and its pyrolysis kinetics are determined using ReaxFF-based molecular dynamics (MD) simulations. The activation energy (E_a) and rate constant (B) of thermal decomposition are obtained as 42.53 kcal/mol and 5.24×10^{12} s^{-1} respectively, using the Arrhenius rate law (Fig. 1a). The results were confirmed to be in agreement with previous TGA experiments and MD simulation studies [1-4]. We use the MD derived kinetics in a higher order mesoscale model to determine the effective surface recession rate of phenolic resin as a function of temperature (Fig. 1b). To extend the analysis to realistic length- and time-scales we propose a continuum level formulation informed by the MD and mesoscale data. We validate the model by direct comparison with previous arc jet and wind tunnel experiments and use it to characterize the AVCOAT TPS [5, 6]. The temperature profile within the AVCOAT TPS, the thickness of resulting char layer as well as the pyrolysis gas blowing rates are calculated for atmospheric re-entry from low-earth orbit and are shown in Fig. 2.

Keywords: Heat shield, Pyrolysis, Phenolic resin, Molecular dynamics, AVCOAT

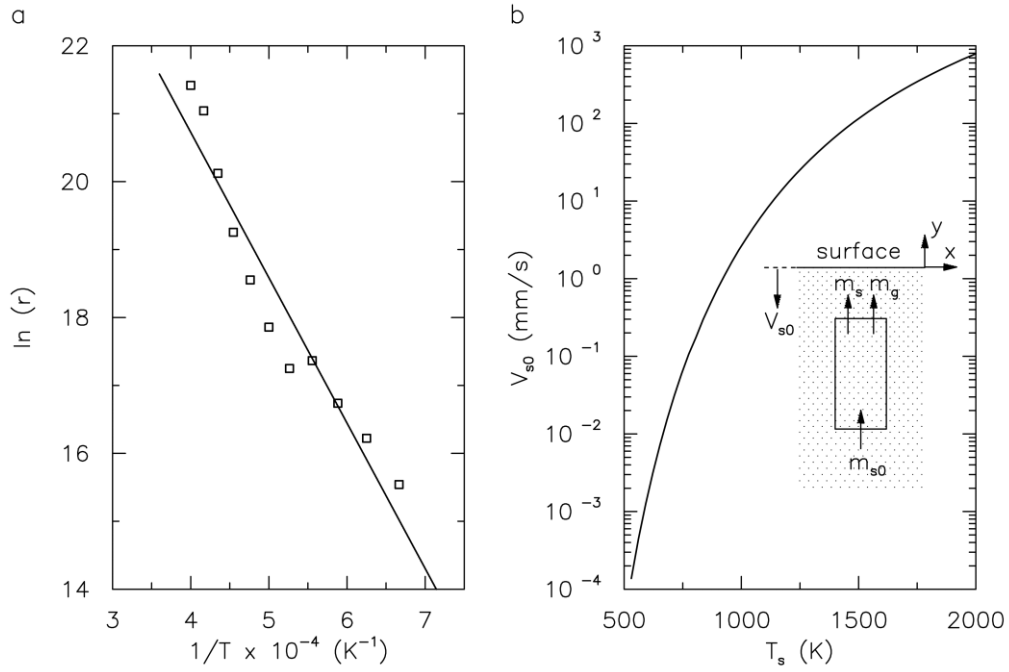

Fig. 1: (a) Arrhenius plot for determination of activation energy (E_a) and rate constant (B) governing the rate of dissociation of C-C bonds during pyrolysis. Symbols denotes the pyrolysis reaction rates from MD simulations at various temperatures. (b) Surface recession rate V_{s0} versus surface temperature T_s induced by pyrolysis of monolithic phenolic resin.

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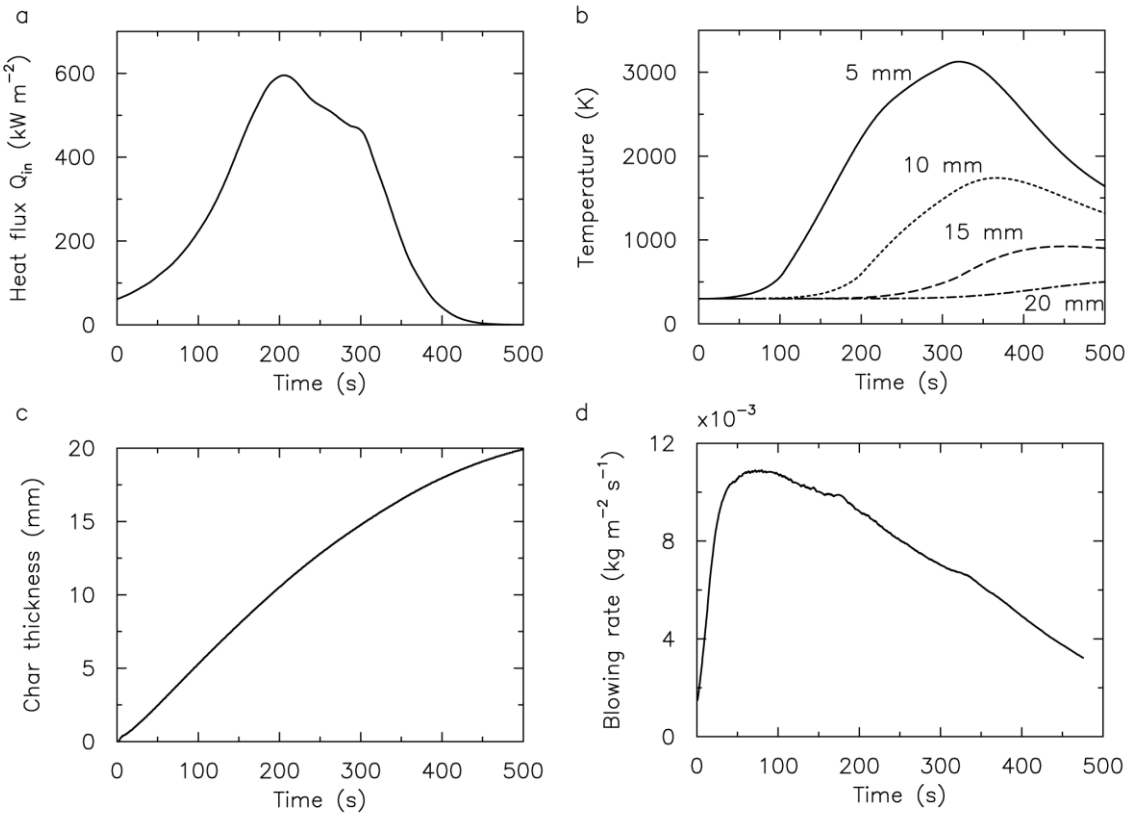

Fig. 2: (a) Time-varying heat flux profile (Q_{in}) experienced by an AVCOAT TPS during atmospheric reentry of a Crew Exploration Vehicle from low earth orbit. (b-d) Predictions of the material response model: Time evolution of temperature at various depths from the surface (b), thickness of the char layer (c), and blowing rate of pyrolysis gases from the surface (d).

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Prediction of TPS material permeability and tortuosity factor using Direct Simulation Monte Carlo

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Abstract

The main objective of this work is to compute the material permeability and tortuosity factor of candidate TPS materials, namely Morgan carbon felt[1] (Morgan Advanced Materials, USA) and FiberForm®[1] (Fiber Materials, Inc.), These materials are composed of a complex shown in Fig. 1. network of carbon fibers of micrometer size on a micrometer scale. Characterizing their material morphology and predicting their permeability and tortuosity factor is critical in modeling the transport of high temperature reentry gases through the material, as well as the material response. We will also obtain the representative elementary volume (REV), so that, material analysis can be performed on smaller samples without compromising on the accuracy of material properties, as well as analyze the effect of material orientation on the material properties. The small characteristic length scale of this problem renders the flow to be rarefied, requiring the use of accurate kinetic theory based approaches known as Direct Simulation Monte Carlo[2] (DSMC). In an effort to improve computational efficiency, we have developed a scalable three-dimensional DSMC solver called Cuda-based Hybrid Approach for Octree Simulations (CHAOS)[3], to accurately model flow through irregular porous media.

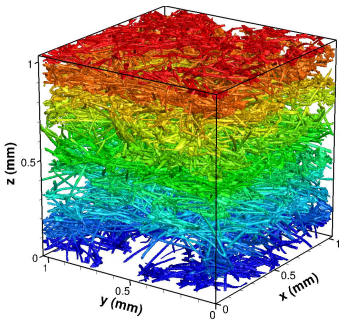

Figure 1: Fibrous microstructure reconstructed from tomography images of candidate TPS materials. Red to blue color scale represents increasing distance from the top surface.

The through-thickness permeability of the felt obtained from CHAOS is compared with the published values from Borner et al[4] in Tab. 1. We observe that the values predicted by CHAOS agree well with the DSMC values published by Borner et al.[4]. Note that the continuum permeability varies by a maximum of 25% when the sample size is varied.

Table 1: Permeability comparison of Morgan carbon felt in the through-thickness (-z) direction

Solver	**CHAOS**	**CHAOS**	**Borner et al.[4]**
Sample size (μ m)	404×404×400	1032×1032×1032	520×520×520
Temperature (K)	2000	2000	310
$K_o \times 10^{-12} m^2$	253	192.4	195

The tortuosity factor, τ_f, is defined as the ratio of the tortuous path length, l_t traveled by the gas particles to the shortest straight path, l, which is also equal to[5]

$$(\tau_f)_i = \frac{l_t^2}{l^2} = \frac{< u >^2}{< u_i >^2} \tag{1}$$

where, $< u >$ is the average speed of the gas particles, and $< u_i >$ is the average value of the velocity component in the i^{th} direction. The tortuosity factor obtained from CHAOS using Eq. 1 for the large 1 mm^3 Morgan felt sample is compared with the continuum regime tortuosity factor computed by Panerai et al.[1] in Tab. 2. It can be seen that the tortuosity factor is higher in the through-thickness direction than the in-plane direction, similar to the trend observed by Panerai et al.[1].

Table 2: Tortuosity comparison for Morgan felt in the through-thickness (-z) and In-plane direction

τ_f	**Through-thickness (-z)**	**In-plane (+x)**
CHAOS (DSMC)	1.16	1.1
Panerai et al. (Continuum)	1.08	1.05

Our preliminary results of material permeability and tortuosity factor for the Morgan felt sample compare well with other published data. To improve the confidence in our results and reduce the error bar, more simulations are needed for both Morgan felt and FiberForm in the through-thickness as well as the in-plane directions. With increase in the number of test cases, we will have the capability to accurately compute the permeability slip factor to account for rarefied flow effects, useful for higher level flow solvers.

Keywords: Permeability, tortuosity factor, TPS materials, DSMC

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Modeling Nonequilibrium Gas-Surface Interactions at High Temperature

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Abstract

The presentation will summarize a new multi-university project, funded by the Air Force Office of Scientific Research (AFOSR), which involves combined experimental and computational research on gas-surface interactions and material response for hypersonic applications. The focus will be on computational modeling of carbon surface ablators (graphite and carbon-carbon composite, for example) as well as silica-based high-temperature ceramic materials. A summary of previous results for oxygen recombination on silica surfaces [1-2] and oxidation on carbon surfaces [3-7] will be presented. Various computational methods will be discussed including molecular dynamics [1-3], direct simulation Monte Carlo (DSMC) [4-6], and computational fluid dynamics (CFD) [7]. A summary of the objectives of the new project, including planned experimental and computational research, will be presented.

Keywords: Ablation, Surface Catalysis, Molecular Simulation

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STM visualization of oxidation reaction kinetics linked with morphological evolution of highly ordered pyrolytic graphite (HOPG) using energy selected supersonic beams of molecular oxygen

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Abstract

The scattering of atomic and molecular beams from well-characterized surfaces is an incisive method for studying the dynamics of gas-surface interactions, providing precise information on energy and momentum transfer as well as complex reaction mechanisms. Scanning probe measurements provide a powerful complement to scattering data as STM and AFM measurements give a direct route to the visualization and spectroscopic characterization of interfacial systems under reaction conditions relevant to ablative systems. We have built a new and unique supersonic beam gas-surface scattering instrument where we combine, in one facility, both reactive scattering and time-sequenced STM/AFM visualization of reacting surfaces. This was initially used to examine the site-specific oxidation of Si(1x1)-(7x7) [1]. We are now using this instrument to study the erosion and ablation of HOPG when exposed to energy selected beams of molecular oxygen. We are observing and linking the reaction probabilities and the morphological evolution of the reacting HOPG (basal plane), with the observation of a variety of structural features including facetted etch pits, direction independent etch pits, and channel formation depending of substrate temperature, defect density, incident beam energy and angle of incidence [2]. Moreover, in support of aerothermodynamic calculations, we have initiated scattering experiments where we monitor velocity and angle distributions for energy transfer and oxidative reaction products, these studies for both basal and prismatic HOPG interfaces. Initial studies involve the energy transfer associated with molecular oxygen and molecular nitrogen from these interfaces as a function of incident angle, incident velocity, and surface temperature. CO and CO_2 products will also be examined in forthcoming measurements. Taken together, our measurements provide an unusually detailed mapping of interface reaction kinetics and energy transfer coupled simultaneously with the morphological evolution of the reacting interface. Surface temperature, impinging O_2 energy and angle affect the morphologies and depth of etch features – vital information for understanding materials erosion and failure.

Keywords: Energetic Oxidation, Reaction Kinetics, Morphological Evolution, Supersonic Beams, STM

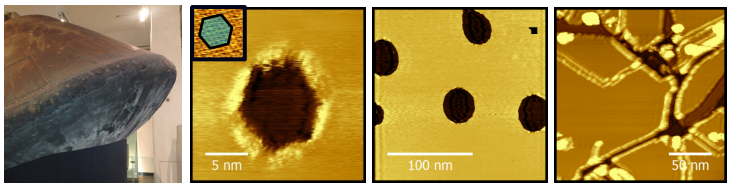

Figure 1: Photo of Apollo 10 ablation shield, photo taken by SJS at The Science Museum of London; HOPG STM resolved molecular oxygen induced etch features, left to right: (i) T_s = 1275 K, θ_i = 0 deg, E_i = 0.4 eV; (ii) T_s = 1375 K, θ_i = 0 deg, E_i = 0.4 eV; (iii) T_s = 1275 K, θ_i = 0 deg, E_i = 0.7 eV.

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High Temperature Carbon Surface Chemistry by Single Particle Mass Spectrometry

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Abstract

In Single Nanoparticle Mass Spectrometry,[1-3] individual particles of a material of interest are trapped in a radio-frequency trap, laser heated, and then exposed to gaseous reactants of interest. Temperature is determined and controlled by measuring emission spectra from the trapped particle. Kinetics for surface reactions are measured by non-destructively monitoring changes in the particle mass, and because the mass precision is high, we are able to measure reaction rates over five or six orders of magnitude. In addition, it is possible to "titrate" the distribution of reactive sites on individual particle surfaces, allowing us to determine reaction/sublimation rates for specific types of surface sites. The method also allows us to explore the particle-to-particle heterogeneity of nanostructured materials. From the ablation perspective, perhaps the most important point is that the upper limit on the accessible temperature range is determined by the sublimation properties of the material, i.e., the more refractory the material, the hotter the technique can go.

The method will be illustrated by results for sublimation and O_2 oxidation of graphite particles.

Keywords: Surface Chemistry, Oxidation, Sublimation

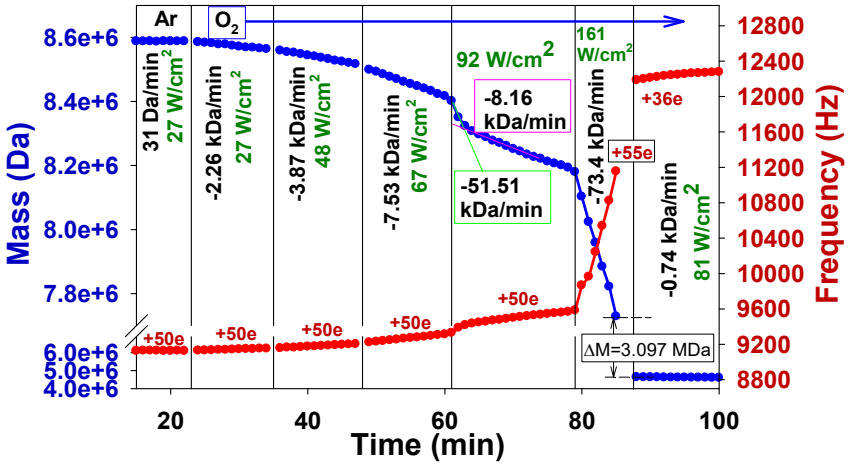

Figure 1: Example Kinetics for oxidation of a single graphite nanoparticle at different heating intensities

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Dynamics of Carbon Oxidation at High Temperatures

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Abstract

This presentation will focus on atomic-oxygen interactions with carbon surfaces relevant to thermal protection systems (TPS). We have studied the interactions of ground-state atomic oxygen, O(^{3}P), on vitreous carbon, FiberForm, and highly oriented pyrolytic graphite (HOPG) at temperatures from 800 K to approximately 2200 K. Beams of 5 eV O atoms were directed at surfaces, and angular and translational energy distributions were obtained for inelastically and reactively scattered products using a rotatable mass spectrometer detector. On all three surfaces, CO and CO_2 are produced at the surface and in thermal equilibrium with it, with CO being the dominant product. The flux of CO reached a maximum on all three surfaces with the peak occurring at different surface temperatures. There was significant thermal desorption of O, which increased with temperature. The increasing thermal desorption of O atoms with temperature limits the surface oxygen that is available for reaction at higher temperatures. With fewer reagent O atoms to react with carbon, the reactivity of the carbon surface decreases at high temperatures even though the surface is being constantly bombarded by highly reactive O atoms [1]. In addition to the competition of O-atom desorption and CO formation, CO formation occurring through three different channels with distinct reaction time scales were identified and characterized from the time-of-flight (TOF) distributions. The molecular-level scattering dynamics from the experiments have been used to formulate a finite-rate oxidation model similar to existing finite-rate models used in computational fluid dynamics (CFD) and direct simulation Monte Carlo (DSMC) simulations.

Keywords: Molecular beam, carbon oxidation

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Ablation of graphitic materials in the diffusion-controlled regime using dynamic non-equilibrium thermogravimetric analysis and oxyacetylene torch testing

Abstract

Carbon 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 literature on oxidation and ablation behaviors of carbon materials, few studies have focused their analysis on the differences in the material microstructures even though reports have been made on how reactivity will influence mass loss rates. In the present work, we investigate the oxidation and ablation behaviors of highly ordered pyrolytic graphite (HOPG), isotropic graphite (I-85) and carbon-carbon composites (C-C) from a microstructural aspect in combine with Thermogravimetric analysis (TGA) and computational fluid dynamics (CFD) modeling, to understand why they react at particular rates under a fixed set of operating conditions. Scanning electron microscopy (SEM) and scanning transmission electron microcopy (STEM) are used for microstructure characterizations on selected specimens. The surface of HOPG (basal plane) is consist of graphite layers of various sizes. Hexagon-shaped pits are observed at tri-junctions or edges of the graphite layers after oxidation. Turbostratic and graphitic structures are observed in the filler material for C-C. Carbon nano-spheres are formed at the tips of the fibers in C-C after oxidation. At temperature below 1300 °C, HOPG and C-C exhibit similar ablation rates, whereas the mass loss rate for I-85 is slightly lower. Despite the structural differences observed, bulk ablation rates are very similar for the three carbon materials during the oxidation test at 1600 °C due to diffusion controlled kinetic reactions controlling rates. Therefore, in order to understand the effect of microstructure and reactivity of graphite materials testing into the rate controlled regime for oxidation kinetics is necessary. Thus, we use the oxyacetylene torch test facility in order to develop an understanding on the effect of graphitic reactivity of the surface under higher flow velocity conditions. The free stream flame environment is characterized as a function of flame chemistry for heat flux, pO_2, and flow velocity. Measured ablation rates for graphite increase as a function of increasing heat flux and pO_2 which are validated by applying an oxygen diffusion based model. The model uses experimentally measured values for temperature, pO_2, and gas velocity in order to confirm torch testing results are reliable and reproducible.

Development of Thermal Conductivity Apparatus for Ablative Composite Materials – an update

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Rafael has developed a transient thermal conductivity apparatus specifically for ablative composite materials. This innovative apparatus is capable of determining thermal conductivity of materials over the temperature range 330 to 1200 k, covering the pyrolytic stage of the composite material. The target specifications of the apparatus are the measurement of thermal conductivity in the range 0.05-5.0 $W \cdot m^{-1} \cdot k^{-1}$ using specimen thickness in the range 7-25 mm. This is achieved using a new design of a symmetric heater-specimen assembly, forcing an adiabatic state along its centerline. The temperature-controlled system is sustained in a closed chamber, capable of introducing specific gases, enabling tests under a wide range of environmental conditions. This device will provide experimental results of thermal conductivity for ablative materials over a wide range of temperatures, enhancing the modeling capability of ablative materials performance in solid motor rockets.

The concept of the device consists of a uniform ramp heating of a composite material specimen, while measuring the temperature difference on both sides of the material. A symmetric assembly of heater-specimen is built up in order to establish an adiabatic boundary condition at the middle interface, assumed according to heat transfer definition. The heat flux to the specimen is measured during the test and the whole device is encapsulated in a blanket with very low thermal conductivity.

The calculated thermal conductivity of the specimen is given by:

$$\lambda_{specimen} = \lambda_{metal} \cdot \frac{\left(\Delta T_{metal} - \beta_0\right) \cdot L_{specimen}}{2 \cdot \Delta T_{specimen} \cdot L_{metal}}$$

Where ΔT_{metal} is the actual temperature difference on the metallic plate , β_0 is the temperature difference on the metallic plate if it were sandwiched as the specimen and had an adiabatic interface, and L is thickness.

Note that this equation is valid if the time duration of the test is greater the summation of the time constants values of the metallic plate and the specimen ($t > [\tau_{specimen} + \tau_{metal}]$).

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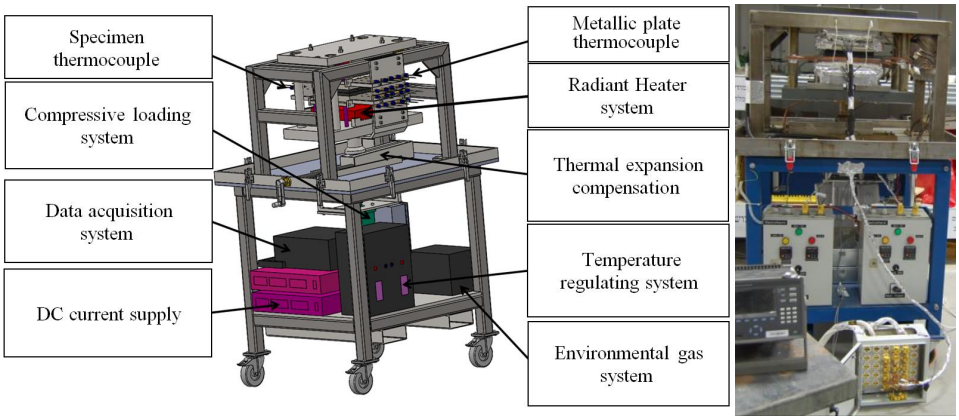

Figure 1. Main features of the transient thermal conductivity apparatus.

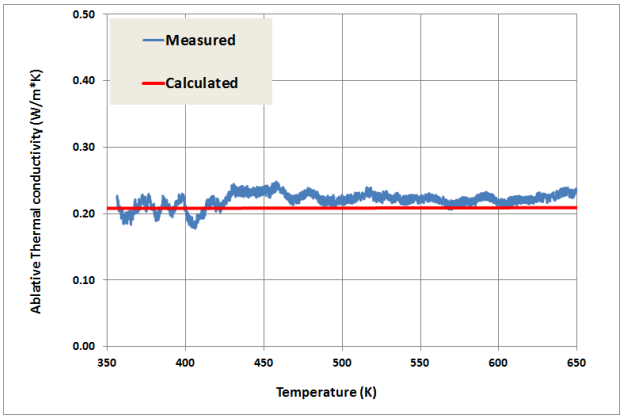

Figure 2. Thermal conductivity of EPDM-based insulation

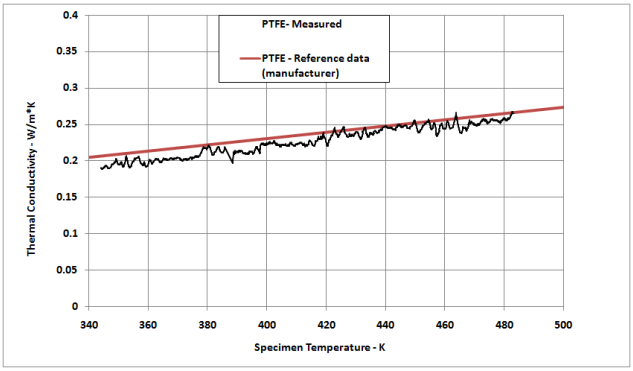

Figure 3. Thermal conductivity of Polytetrafluoroethylene (PTFE)

The Kentucky Re-entry Spacecraft (KRUPS) for TPS Testing: Overview of SRF-1

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Abstract

The design of an efficient Thermal Protection System (TPS) remains one of the most challenging tasks of planetary exploration missions. Because of the harshness of re-entry environments, ground tests cannot replicate these conditions. Consequently, engineers must rely on numerical models that often lack validation data. To provide a path toward inexpensive validation, the Kentucky Reentry Universal Payload System (KRUPS) spacecraft is being developed at the University of Kentucky.

A KRUPS spacecraft is being released from two separate sounding rocket launches (KUDOS and KOREVET) at 150 km to obtain data for the TPS as the technology matures toward the eventual goal. KUDOS launched on August 12, 2017, and KOREVET is set to launch in March 2018. These launches are an important step toward the next phase, releasing a KRUPS test article from the International Space Station (ISS). They are expected to raise the Technology Readiness Level (TRL) to TRL 6 by demonstrating data acquisition, communication, sensing, and TPS designs, demonstrating readiness for release from the ISS.

Keywords: Thermal Protection System (TPS), Ablation, Computational Fluid Dynamics (CFD), Sounding Rocket, International Space Station (ISS), Reentry

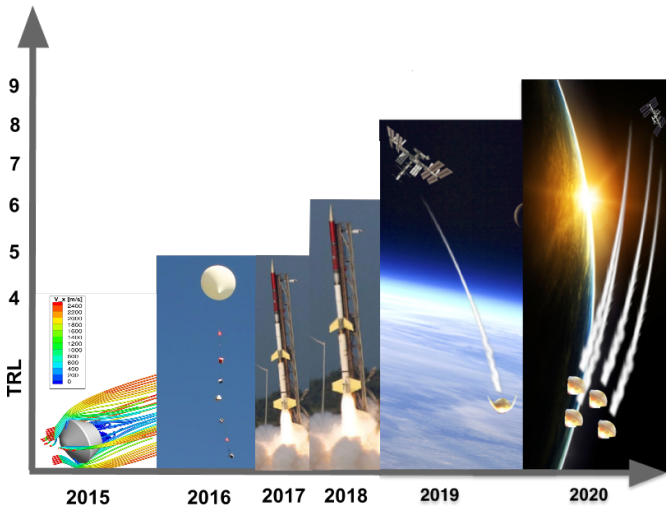

Figure 1: The TRL roadmap for KRUPS project

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Thermal Decomposition of PICA at Heating Rates Relevant to Flight Conditions

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Abstract

The thermal decomposition of phenolic impregnated carbon ablator (PICA) has been investigated with the objective of measuring molar yields of pyrolysis products at heating rates that are relevant to MSL flight conditions. Specifically, PICA has been pyrolyzed at heating rates of 3.1, 6.1, 12.7 and 25 °C s^{-1}, that spanned a temperature range of 100-1200 °C. Samples were restively heated in a differentially pumped vacuum chamber and pyrolysis gases were measured with a carefully calibrated mass spectrometer. The relative molar yields of 14 pyrolysis gases were obtained in conjunction with mass loss measurements. These measurements allowed for the calculation of absolute molar yields and mass yields as a function of heating rate, as well as the simulation of TGA curves. Pyrolysis product yields change as a function of heating rate, and this behavior has been attributed to two mechanisms that compete during the initial stages of thermal decomposition. The first reaction involves the condensation of hydroxyl functional groups to form carbon-carbon bonds or ether functional groups. The second reaction involves the breakdown of the methylene bridge between phenol monomers to yield phenol and its derivatives. The second decomposition reaction dominates at higher heating rates. The results of this study are now available for use in material response models.

Additionally, we have developed an experimental methodology that allows us to pass a model gas through a hot carbon preform sample and measure reaction products as a function of time and temperature. Our most recent efforts to investigate the reaction of molecular oxygen with preform and charred PICA samples up to 1800 °C will be presented.

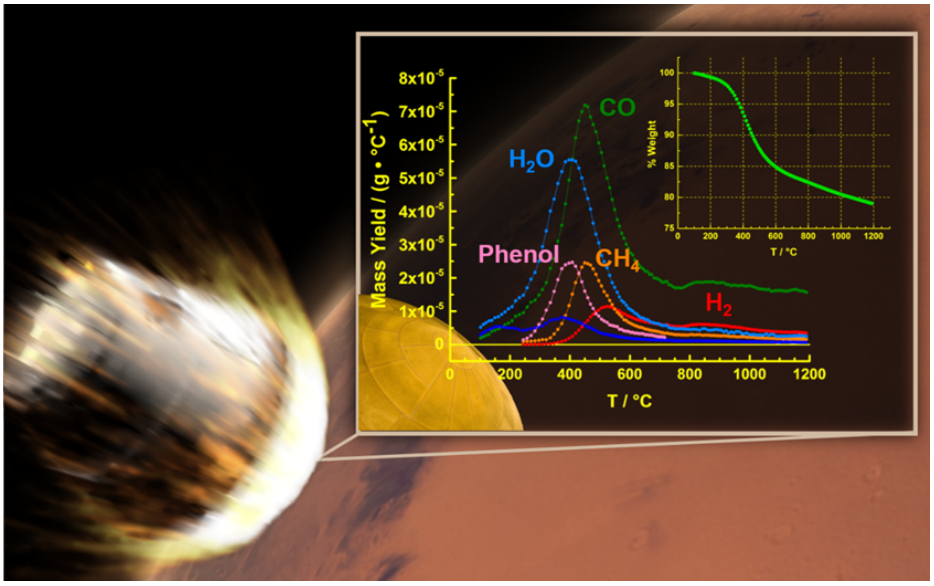

Figure 1: Mass yields of PICA pyrolysis products and simulated TGA at a nominal heating rate of 3.1 °C s^{-1}.

3D Material Response Analysis of PICA Pyrolysis Experiments

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Abstract

The PICA decomposition experiments of Bessire and Minton [1] are investigated using 3D material response analysis. The steady thermoelectric equations have been added to the CHAR code to enable analysis of the Joule-heated experiments and the DAKOTA optimization code is used to define the voltage boundary condition that yields the experimentally observed temperature response. This analysis has identified a potential spatial non-uniformity in the PICA sample temperature driven by the cooled copper electrodes and thermal radiation from the surface of the test article (Figure 1). The non-uniformity leads to a variable heating rate throughout the sample volume that has an effect on the quantitative results of the experiment. Averaging the results of integrating a kinetic reaction mechanism with the heating rates seen across the sample volume yield a shift of peak species production to lower temperatures that is more significant for higher heating rates (Figure 2) when compared to integrating the same mechanism at the reported heating rate. The analysis supporting these conclusions will be presented along with a proposed analysis procedure that permits quantitative use of the existing data. Time permitting, a status on the in-development kinetic decomposition mechanism based on this data will be presented as well.

Keywords: Pyrolysis, PICA, Heat Transfer, Non-Equilibrium, CHAR, Thermoelectric

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URL `http://dx.doi.org/10.1021/acsami.7b03919`

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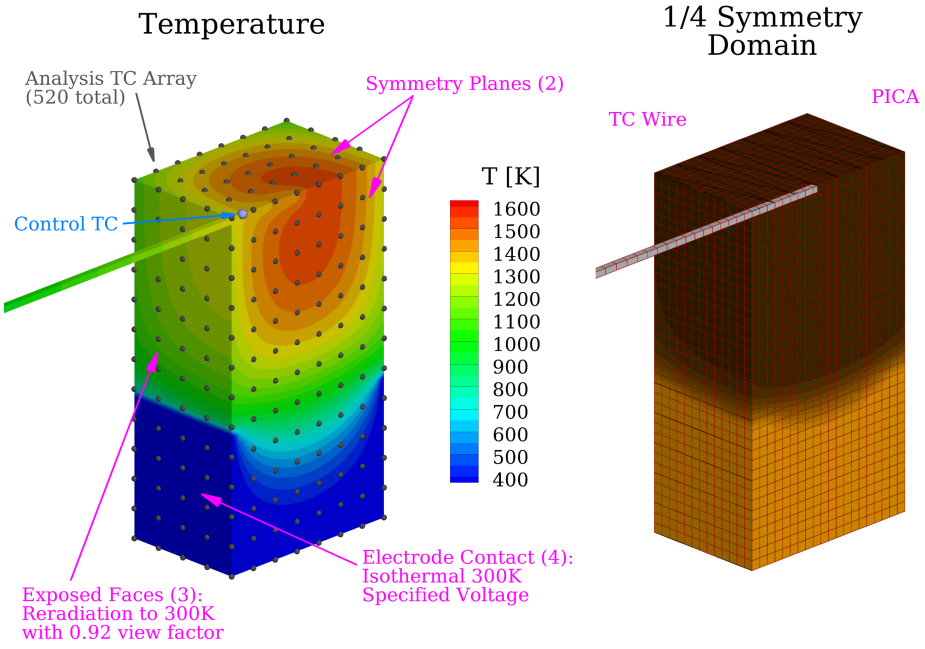

Figure 1: Computational domain and temperature field at end of 25 K/s run.

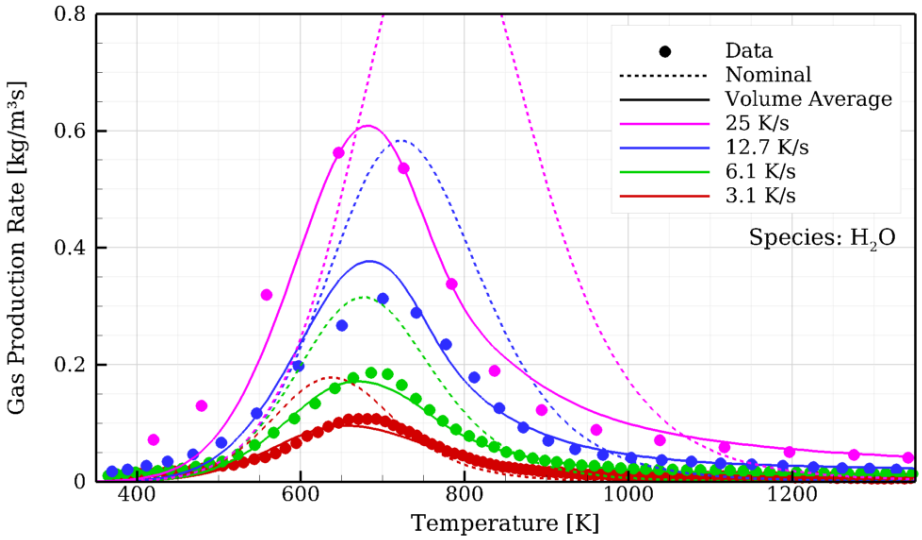

Figure 2: H_2O gas production rate for Arrhenius model integrated at reported heating rate (dashed lines) and the volume-averaged integration of the same Arrhenius model (solid lines) compared to measured data. Colors denote different reported heating rates.

Using Bayesian Inference in the Calibration of VISTA Material Database

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Abstract

The current design of NASA's Multipurpose Crew vehicle utilizes newest revision of the AVCOAT charring ablator. The re-emergence of this material has brought about the need to improve current methodologies used in predicting TPS material performance in flight. A research group at University of Kentucky has developed the open-source VISTA charring ablator material model based on Apollo-era AVCOAT data available in past publications. In this work, we calibrate uncertain parameters of the VISTA material model using Bayesian inference and data collected during the Apollo 4 test flight. Prior to performing the calibration, a sensitivity study is done using two commonly seen methods in published works, Pearson correlation coefficients and the method of Sobol. The results of both approaches are compared and the applicability of each is evaluated in the context of models meant to predict material response of charring ablators. Following, exercises in the calibration of influential uncertain parameters of VISTA are performed from Bayesian statistics point of view where uncertainty due to parametric, model, and data sources are quantified. A case with generated synthetic data is first studied where the obtained results validate the methodology applied in this work as well as confirm the ability to retrieve parameter values from the current scenario. Uncertain VISTA model parameters are then calibrated using Apollo 4 material temperature flight data. In the final step, quantified parametric, model error, and data inaccuracy uncertainties are propagated onto the model output where it is expressed as a probability distribution function, and a large decrease in uncertainty is observed.

Keywords: Uncertainty Quantification, Bayesian Inference, Calibration, TPS, Bayes Theorem, VISTA

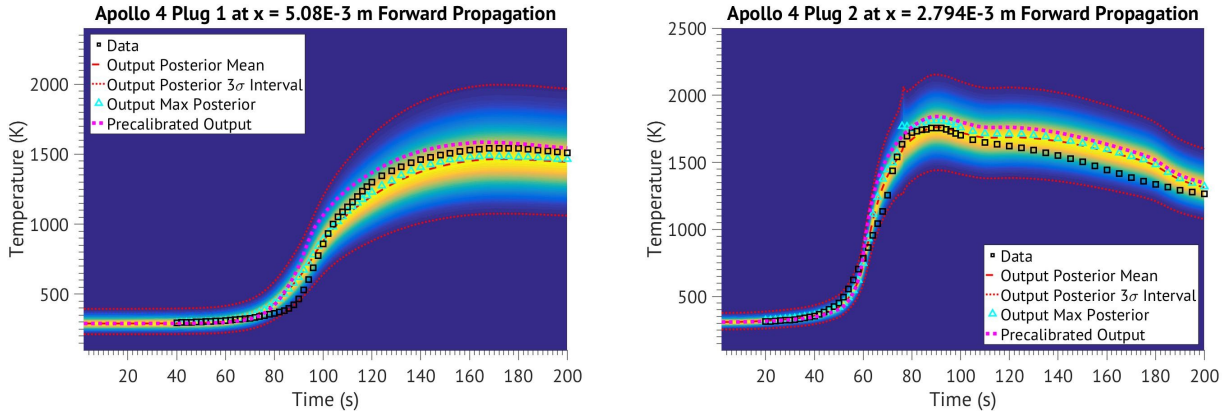

Figure 1: The solution of the statistical forward problem where quantified uncertainties associated with parametric, model, and data sources were forward propagated onto the model output quantity of interest for two thermocouple locations, separately in Plug 1 (a) and Plug 2 (b).

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Conjugate Analyses of Ablation in Rocket Nozzles

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Abstract

This presentation will describe progress towards performing conjugate analyses of ablation in rocket nozzles. The conjugate analysis methodology being developed in this effort couples the LeMANS [1, 2] flow solver to the multi-dimensional MOPAR-MD [3, 4] ablation and material response code. Results from conjugate analyses of the HIPPO nozzle test case are compared to a baseline analysis following a traditional, decoupled approach.

For conjugate analyses, the flowfield and material responses are computed in a closely-coupled manner, in order to capture mutual interactions. The pressure trace for a rocket motor firing is divided into a number of discrete time points; the LeMANS flow solver is used to obtain a steady-state flowfield solution at each point. The wall boundary conditions required by the flow solver (temperature, injected mass flux, wall displacements) are obtained from MOPAR-MD, which is linked to the flow solver as a boundary condition routine. At each time point, MOPAR-MD performs a transient material response analysis starting from the solution obtained at the previous time point, using convective heating conditions passed from the flow solver. Smoothing is applied to values passed between the flow and ablation response solvers to suppress instabilities associated with perturbations in the ablated nozzle contour. The LeMANS flow solver and the MOPAR-MD material response solver work in an iterative fashion, with MOPAR-MD being called at intervals based on a heat flux convergence metric.

Five different treatments of the surface energy balance at the ablating wall, with increasing levels of fidelity, are investigated. The Noncatalytic Wall – Heat Flux (NCHF) treatment uses a noncatalytic wall boundary condition for the flow solver, and passes a raw flux to the material response solver. It greatly over-predicts heat flux and surface recession, and is found to be inappropriate for rocket nozzle applications, even though it has been used for external TPS applications [5]. The Noncatalytic Wall – Enthalpy Conductance (NCEC) method is an improvement that passes enthalpy conductance instead of raw heat flux. For the Ablating Wall – Heat Flux (AWHF) and Ablating Wall – Enthalpy Conductance (AWEC) methods the species mass fractions at the walls are specified according to the equilibrium composition, providing increased fidelity to the flow solver calculations. The Integrated Equilibrium Surface Chemistry (IESC) treatment computes the surface energy balance directly from the diffusive fluxes at the ablating wall, without making transport coefficient assumptions or requiring pre-computed B' tables. The IESC method provides the highest level of fidelity, and can inherently account for the effects of recession, wall temperature, blowing, and the presence of ablation product species in the boundary layer.

Predicted surface recession distributions for the HIPPO nozzle at $t = 2.0$ s are compared in Fig. 1. Clearly, surface recession is strongly affected by the choice of surface energy balance treatment, while surface temperature (not shown) is less sensitive. The lowest surface recession is predicted with the IESC method, and extrapolating these preliminary results suggests that the IESC treatment will provide improved agreement with experimental data. Simulations are in progress for the full duration of the HIPPO motor operation, which will enable a proper assessment of the various modeling approaches.

By solving the ablation problem in a fully conjugate manner, the strong interactions and interdependencies that exist between the reacting flowfield and the ablating material are captured rigorously, and many of the simplifying assumptions that must be made in decoupled ablation modeling approaches are avoided. This places the analysis more strongly upon first principles, and should improve the accuracy of the resulting predictions.

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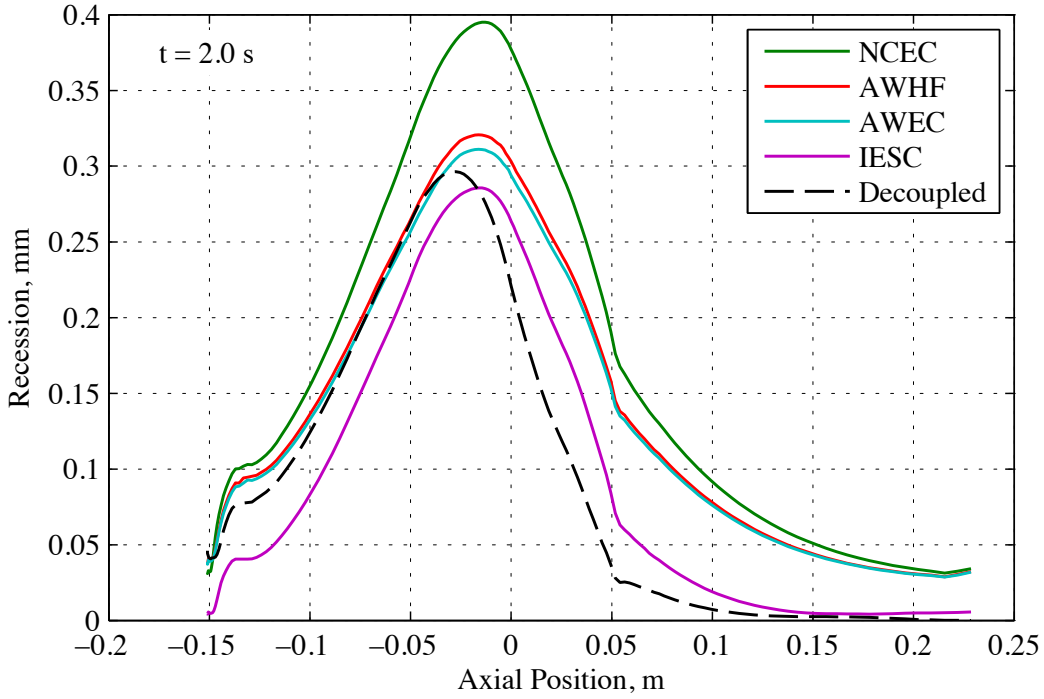

Figure 1: Surface recession distribution within the HIPPO nozzle at $t = 2.0$ s, as computed by the decoupled analysis and by conjugate simulations using the different surface energy balance approaches.

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Numerical Modeling of Ablation Materials in Solid Rocket Motors

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There are different kinds of ablation materials which protect rocket cases from thermal loads. Degradation of ablation materials is explained with two main ablation mechanisms. To well understand the mechanism of ablation, Figure 1 can be examined. During the degradation of the erosion surface of EPDM (ethylene propylene diene monomer), a region called pyrolysis zone is formed. In this region, chemical reactions occur and a char layer forms.. At the surface of the ablation material, thermal and velocity boundary layers are influenced by the products of the pyrolysis. This affects the heat transfer rate between the hot gases and the insulation material.

This work deals with modelling of ablation mechanism of the surface of the insulation material called EPDM subjected to the hot gases in a rocket combustion chamber. In order to model degradation of surface of the EPDM, a commercial code (Ansys/Fluent) was used. The capabilities of the Fluent solver to resolve the boundary layer region near the ablation material surface was investigated and it was concluded that the wall functions should be modified by considering the pyrolysis gas blowing effects. For this reason, a UDF (user defined function) was developed and adapted to the solver. By using the experimental data of a literature test case [2], developed heat transfer model is tested and it was seen that numerical results are not so good aggrement with the test data. Then for the future work, it was decided that chemical reactions effects must be taken into account and should be solved by another UDF.

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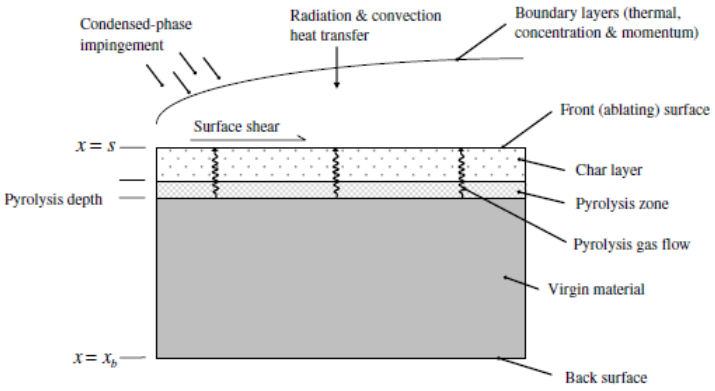

Figure 1 Phenomena [1]

Development of DSMC Surface Oxidation Model for Carbon from Analysis of Molecular Beam Experiments

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Abstract

Computational modeling of molecular beam experiments of a hyperthermal oxygen beam striking a vitreous carbon surface is performed using direct simulation Monte Carlo (DSMC). First, a detailed surface reaction framework is developed in the DSMC solver SPARTA [1], which includes adsorption, desorption, Langmuir-Hinshelwood (LH) mechanisms, etc. The probabilities and the characteristic time scales of the reaction mechanisms are computed based on the reaction rate constants, sticking coefficients, surface properties, and instantaneous coverage. This framework also incorporates microscopic information regarding the detailed scattering of the products (including desorption barriers, angular scattering), in addition to the macroscopic information (reaction mechanisms, rate constants) [2]. This framework is used to numerically simulate the beam scattering experiments of oxygen on a vitreous carbon surface [3] over a range of surface temperatures from 600-2000 K. A detailed study is performed to examine the time-of-flight (TOF) and angular distributions corresponding to the various reaction mechanisms under a range of conditions [4]. The results of this study are used to analyze the experimental TOF distributions and propose modifications to the carbon surface oxidation model developed by Poovathingal and co-workers [5]. This revised model captures the important features in the experimental TOF distributions, including the impulsively scattered (IS) and thermally desorbed (TD) components in the O TOF distribution, and the relatively slow components in the long tail of the CO TOF distribution. Figure 1 presents the comparison between the simulated DSMC TOF distributions (computed using the revised finite rate model) and experimental TOF distributions for both O and CO at 800, 1000 and 1875 K. The angular distributions and relative product fluxes are also observed to be in excellent agreement with the experiments [6].

Keywords: DSMC, Surface Chemistry, Carbon Ablation, Oxidation, Gas-Surface Interaction.

Acknowledgements

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

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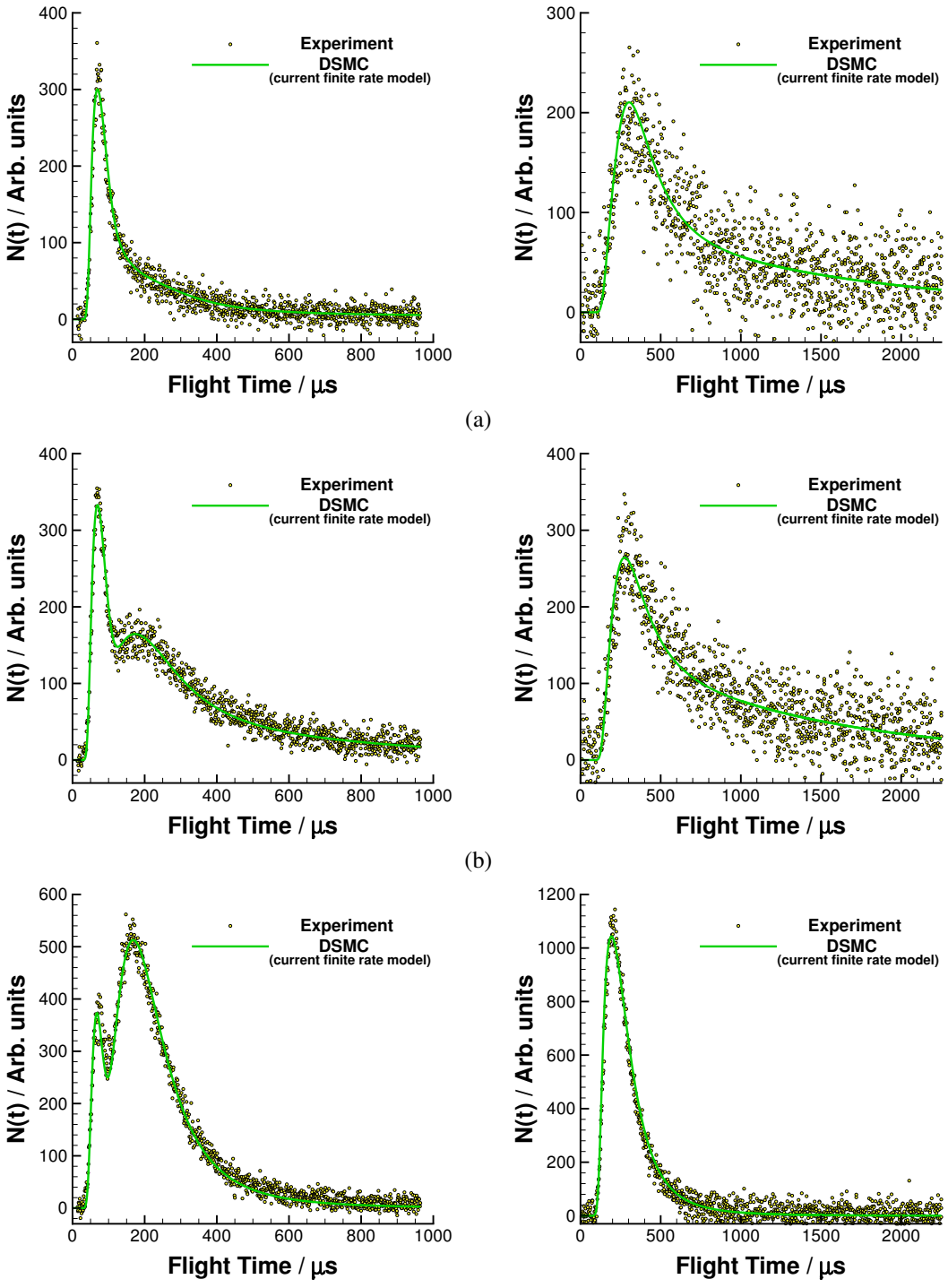

Figure 1: Comparison of TOF distributions at $\theta_f = 45^o$ of O (left), and CO (right) obtained from DSMC with the derived finite rate model and the results from the molecular beam scattering experiments [3] at (a) 800 K, (b) 1000 K, and (c) 1875 K following bombardment with the oxygen beam on vitreous carbon at $\theta_i = 45^o$.

Carbon Oxidation in Extreme Environments

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Abstract

Carbon-based materials are often used in Thermal Protection Systems (TPS) in Hypersonic aircrafts applications. They stand well high temperatures but the TPS protective potential can be compromised as carbon gasifies in the presence of oxygen and high temperatures. Thus, reliable predictive oxidation models are an important component in TPS design.

The common current approach to carbon oxidation is to use available experimental results to adjust the reaction rates of an educated guess oxidation mechanism, involving a number of intermediate steps and species. The mechanism proposed by Shaddix' group[1], is a reasonable balance between accuracy and complexity. We have successfully used it to model the oxidation of porous fiber-based materials in order to understand how flow parameters such as the mass flow rate or ambient pressure and temperature determine the transition between surface and volumetric ablation. We discuss extensively these results and how they can be used in the design of Thermal Protection Systems using these kind of materials.

There are however fundamental methodological limitations to these type of phenomenological kinetic schemes that seriously restrict their potential use as predictive tools. They reproduce well experiments but they can not reliably be used beyond the experimental conditions of the data they are based on. We discuss these limitations, their source and possible remedies.

Keywords: TPS, Hypersonics, Carbon Oxidation, Porous Materials, Homogenization

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Particle methods for tortuosity factors in porous media

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Abstract

Accurate modeling of diffusion-reaction systems, for example the in-depth oxidation of carbon fiber thermal protection system (TPS) materials, requires an understanding of how the porous media resists a diffusive flux. A common model for diffusive transport uses the concept of a tortuosity factor, a value that quantifies the diffusive resistance of a porous media. In the continuum regime, finite-volume schemes can be used to solve Fick's law of diffusion and compute the effective diffusivity and tortuosity factor in porous media. In the transitional and rarefied regimes however, these approaches are no longer valid and particle based methods provide a better approach to model the physics of diffusive transport.

In this work, we implemented and studied a random walk method to compute the effective tortuosity factor in porous and fibrous media. We compared the method to results obtained using the Direct Simulation Monte Carlo (DSMC) technique. The random walk method was implemented into the Porous Materials Analysis (PuMA) [1] software, following the formulation of Tomadakis and Sotirchos [2]. Simulations at different Knudsen regimes were performed by changing the mean free path of the random walks. The free path of a given particle trajectory was modeled with a Maxwell-Boltzmann distribution centered around the mean free path. Diffuse reflections were used for surface collisions and a mean square displacement method was used to determine the effective diffusion coefficient in the porous media. Reflective boundary conditions were used, which provided sufficient accuracy for random porous media. It was found that in the transitional and rarefied regimes, a cuberille surface cannot be used and the surface collisions must be determined based on an iso-surface approximation, such as that produced by the marching cubes algorithm [3].

In the implemented model, the reference diffusion coefficient is taken to be the diffusion through a capillary with a diameter equal to the porous medium characteristic length, a method popularly adopted in the literature. The limitations of this model were investigated.

The results of the random walk method were compared to DSMC simulations using the SPARTA[4] code. The simulations in SPARTA were run in argon and the influence of the Knudsen number was studied by varying the pressure. The DSMC and random walk methods showed good agreement at all Knudsen regimes.

Keywords:
Diffusivity, Tortuosity, Continuum, Rarefied, Porous Media

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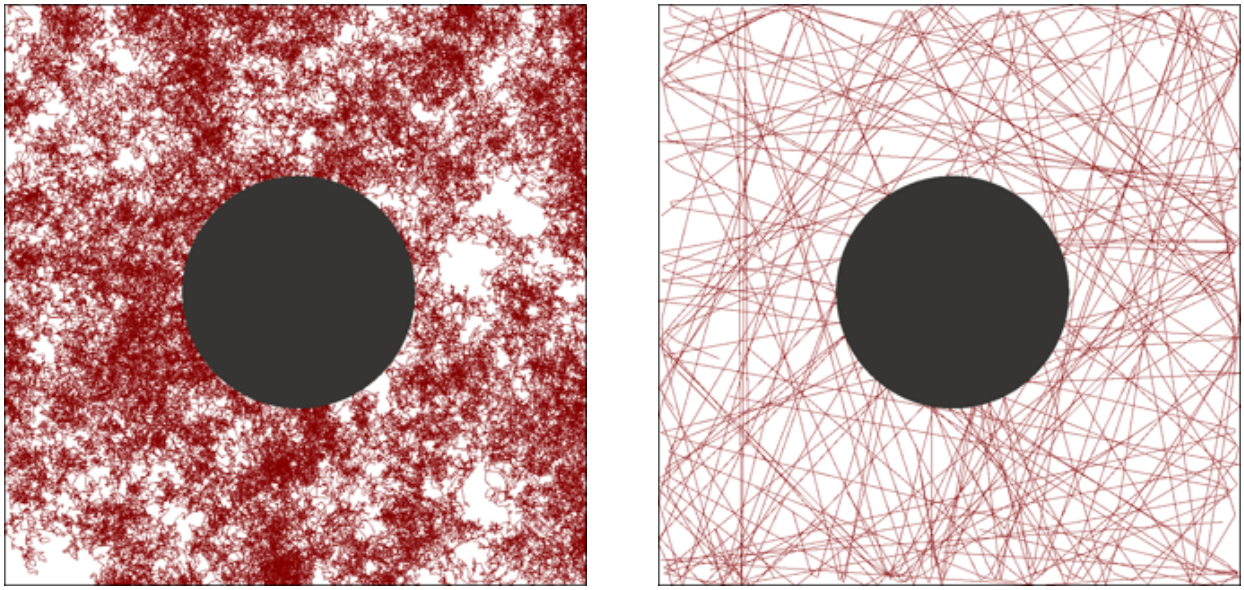

(a) Low Knudsen number

(b) High Knudsen number

Figure 1: Visualizations of PuMA random walks in a periodic collection of cylinders. Red lines show particle paths.

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In-situ Ablation Sensor and Numerical Modeling of Three-dimensional Woven Carbon/Phenolic Ablative

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Extended Abstract

A three-dimensional woven carbon/phenolic (3D C/Ph) ablative manufactured by Airbus Safran Launchers, Le Haillan, France has been studied to gain insight to the material's internal and surface behaviors under severe heating environment. Airbus Safran Launchers utilizes this 3D C/Ph material for use in solid rocket motor (SRM) nozzle designs. An oxy-acetylene flame was applied to the surface of the 3D C/Ph ablative to simulate a medium heat flux of 350 W/cm^2 for a test duration of 100s under a non-oxidative test environment. The "In-situ Ablation Sensor" technique, a real-time ablation measurement technique developed by the Koo Research Group [1, 2] offers a new means to obtain data economically, was implemented in this study (Fig. 1). This well-established measurement technique allows the recession rate of the 3D C/Ph material to be characterized electronically, while simultaneously recording the ablative's internal temperature profile during flame exposure. The surface behavior of the ablative was also characterized using advanced diagnostics by utilizing a two-color Infrared (IR) pyrometer, IR video camera, and high definition (HD) video camera. Through the usage of these measurement devices, an optical as well as an electronic ablation rate and surface behaviors of this novel 3D C/Ph ablative were investigated under realistic conditions. This study also details an ongoing investigation with the objective of establishing the "In-situ Ablation Sensor" as an effective method for monitoring the health of solid rocket motor (SRM) ablative materials, such as the 3D C/Ph material through experimentation supported by numerical modeling.

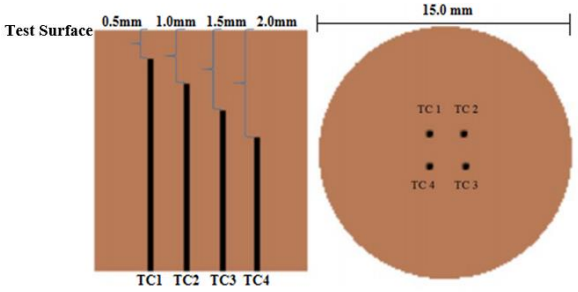

Fig. 1 Holes drilled for in-situ ablation sensor.

Ablative Behavior Analysis

Figure 2 is a representative of the camera data obtained during each of the performed ablation tests. In theory, the HD camera allows for the possibility to calculate an optical ablation rate by recording the time at which a hole appears in a specific frame [4]. This frame is then used to calculate a rate of recession based on the time of the frame and the known depth of the hole from the embedded thermocouple. In all three tests, no holes appeared on the test surface of the samples tested; however, the HD and IR cameras were used to gain insight into the C/Ph testing process.

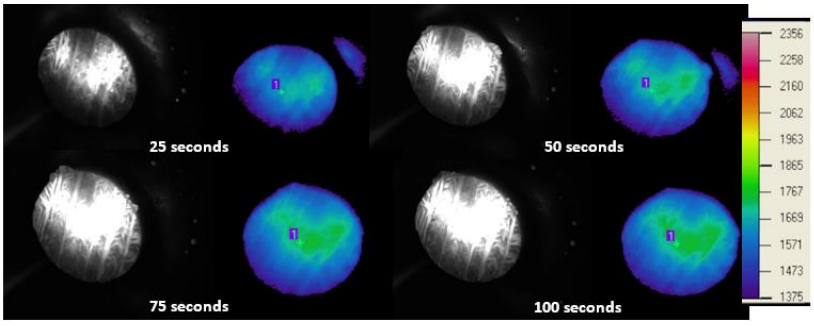

Fig. 2. Test 3 IR and HD cameras close-up images.

In addition to depicting the test surface temperature profiles, the images also reveal the accuracy of the torch tip and location where the flame was applied. During the first and final ablation tests, the C/Ph saw the most centered positioning of the torch tip. The torch tip's location relative to the test surface caused the embedded thermocouples positioned in the center of the samples to experience a more direct source of heat transfer compared to the second test. The IR pyrometer, also directed at the center of each test sample, recorded higher surface temperatures for the first and final

tests in comparison to the second test. The third test's internal temperature profile reached the highest temperatures recorded by the TCs in comparison, which appears to have the most central positioned flame. The position of the torch tip and flame could help explain some of the interesting internal phenomena that occurred during the first and third tests.

Ablation Recession

The in-situ thermocouple technique failed to record ablation data for all samples tested due to the C/Ph ablative's resilience to the 350 W/cm^2 heat flux during each of the 100 second test cycles. This is also true for the data derived from the HD camera. The in-situ technique records ablation by revealing at which point in time each of the incrementally positioned thermocouples break at their known distances. An ablation rate is found through the HD camera frames by providing an accurate point in time where the thermocouple hole becomes visible in frame. The ablation was estimated using a pair of calipers to calculate the change in specimen length before and after testing. Although, this is not the most accurate way of measuring recession, these measurements give an idea of what the 3D C/Ph material's theoretical ablation rate could be. Because of the straight-edged nature of the calipers, certain features of the test surface such as grooves, crevices, and indentions are not taken into account. In using this caliper measurement process, the average ablation rate was found to be estimated at approximately 1.8 μm/s [4]. An additional set of three experiments with TC locations closer to the front surface of the sensor is in progress.

Numerical Analysis

A numerical model provided by Airbus Safran Launchers using a propriety code shows a thermal calculation in comparison to the data collected from the second test sample's result. In the modeled 3D C/Ph sample, a thermal calculation was performed by applying the measured surface (wall) temperature provided by the IR pyrometer's experimental data. In addition to applying the recorded surface temperature, the thermocouple closest to the test surface was moved to a position located 400 μm from the test surface. The results of the thermal calculation have been superimposed on the existing data from the IR pyrometer and in-situ thermocouples for the second test cycle.

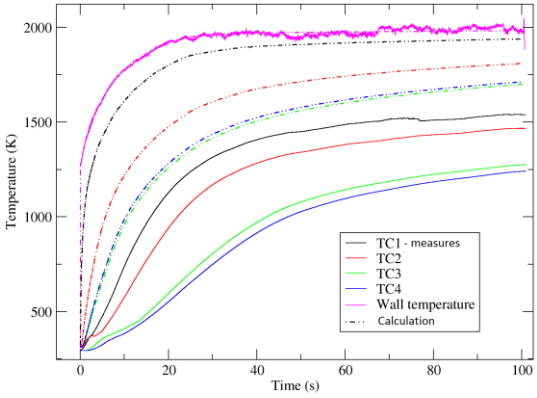

Fig. 3 Calculation at temperature imposed on Test 2.

Figure 3 shows that once the surface temperature is applied to the calculation, the thermocouple closest to the test surface approaches the same temperature as the wall temperature. The results of the numerical analysis are far from the internal temperature measurements, thus pointing out the discrepancy between the surface temperature measurements from the IR pyrometer and thermocouple data. This inconsistency could be due to the response time of the thermocouples being slower than the instantaneous radiative pyrometer, causing the predicted temperatures to be well above the measurements. Despite this difference, the analysis fit well in comparison to the surface temperature as the surface temperature is the only temperature that influences ablation. Additional numerical modeling effort is in progress using new ablation data.

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Interaction of ablating carbon with expanding Earth entry flows in the X2 expansion tube

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Abstract

The atmospheric entry of a spacecraft is characterized by very high entry velocities which give rise to harsh conditions behind the bow shock wave in front of the vehicle. In case of ablative thermal protection system (TPS), the associated heating and shear force from the very high flow speeds result in ablation of the TPS material. The ablated products become entrained in the flow and travel further downstream which influences the heat transfer to the afterbody of the vehicle. The ablation and pyrolysis products could be both absorbers or emitters of radiation depending on the conditions, and accordingly, radiation blockage or radiation enhancement could occur. The uncertainty associated with the estimation of the afterbody heating lies around 50–300% [1] and it leads to large safety factors in TPS design. In the present work, this ablation product entrainment into the expanding re-entry flow is simulated by electrically heating graphite strips to temperatures ranging from 1800–2400 K and exposing them to Earth entry flow conditions generated by the X2 expansion tube at The University of Queensland, Australia. The method of electrical pre-heating for hot wall testing in hypersonic impulse facilities was established by Zander [2], and is adapted for the present graphite ablation experiments in X2. The graphite strips are located on the compression face of a 2D wedge as shown in Figure 1. These experiments are aimed to seed the high speed flow with ablation products and to study their evolution and interaction with the flow downstream. The flow is characterized by ultraviolet emission spectroscopy in both the shock layer and downstream expansion region as illustrated in Figure 1, at three different heights above the wedge model: planes of sight at 0.75 mm, 4.0 mm and 6.5 mm from the model surface.

A high speed video frame is shown in Figure 2, which shows the shock layer, expansion fan and the ablation of graphite particles into the flow. The heated graphite strip temperatures are estimated using dual-wavelength thermography. Results from an example test case are shown in Figure 3 for which the graphite is heated to around 2200 K and the plane of sight is at 4.0 mm above the wedge model. The spectral image shows the radiation from species emitting from the shock layer and expansion. Appreciable emission is observed from the CN radical which is formed by interactions between the ablated carbon and dissociated air. The emission from a concentrated CN band is averaged (region between lines 1 and 2) and the resulting spatially resolved spectral radiance shows the distribution of CN radicals in the flow downstream. The emission from the shock and expansion is averaged (region between lines 3 and 4) and the resulting wavelength resolved plot is also shown in Figure 3. The emission from aluminium contaminants, originating from secondary diaphragm, is also seen in the spectra. Results of other temperature cases and at other planes of sight in the flow will also be discussed.

Keywords: Carbon ablation, Radiation, Earth entry flows, X2 expansion tube, Ultraviolet emission spectroscopy

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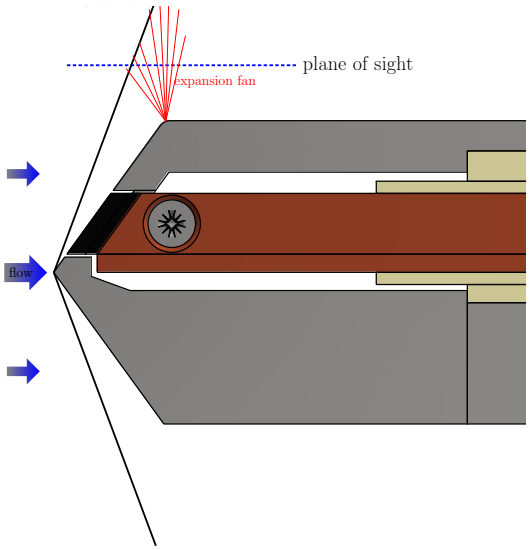

Figure 1: Schematic illustration of electrically heated graphite strip mounted onto the compression face of a wedge model under Earth entry flows. Spectrometer plane of sight above the wedge top surface.

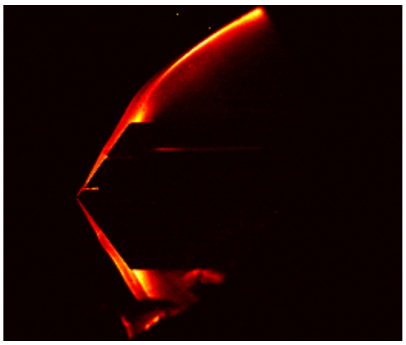

Figure 2: High speed camera image showing ablation particles and flow features during test time.

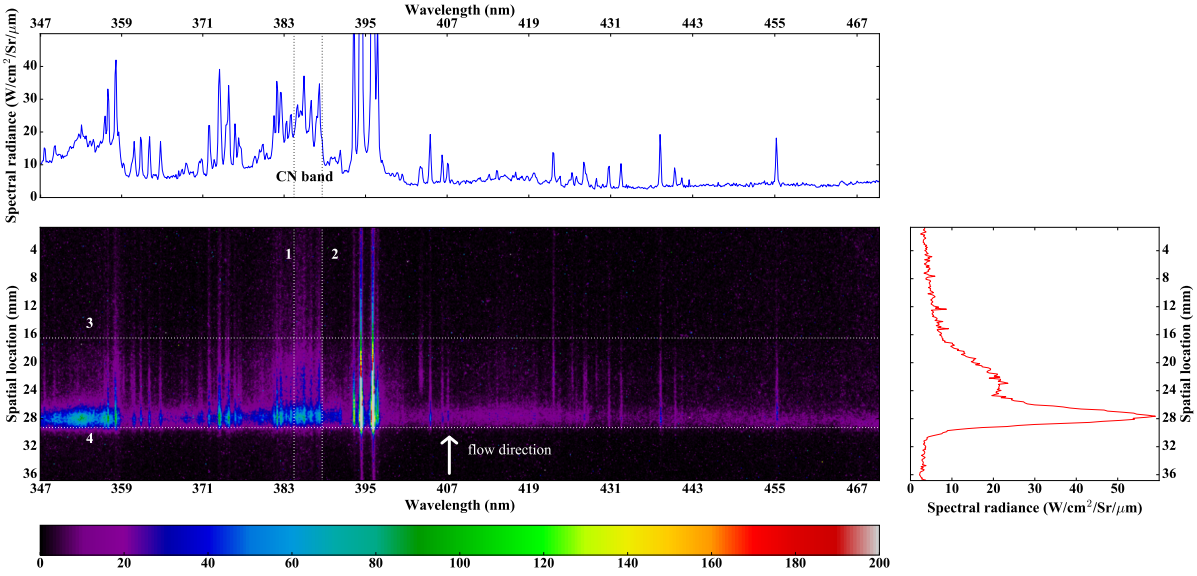

Figure 3: Ultraviolet emission spectrum covering the shock layer and the expansion downstream, from a plane of sight at 4.0 mm above the wedge model. Emission from CN is observed in both the shock layer and expansion fan. The spatially resolved spectral radiance plot is averaged between the lines 1 and 2, and the wavelength resolved plot is averaged between the lines 3 and 4.

Ablation experiments of the ZURAM carbon-phenolic ablator for test case definition and material code validation

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Abstract

We study ablation, pyrolysis outgassing, and thermal response of the carbon-phenolic light-weight ablator ZURAM, which was developed at the DLR for aerospace applications as well as for academic studies and research projects. The ablation tests of ZURAM samples of hemispherical shape with 25 mm radius have been carried out in the high-enthalpy Plasmatron ICP facility at the VKI. Until now, ZURAM is not covered with ITAR or export license restrictions and presents an ideal candidate for producing experimental data to be internationally shared for ablation test case definition.

The primary goal of the experiments was the generation of a database for validation of numerical material response tools at VKI and with collaborators. All samples were equipped with 7 thermocouples at different radial and axial locations, with their in-depth position determined with high accuracy by 3D X-ray microtomography. The stagnation point surface temperature was measured by two radiometers and a surface temperature map has been created with an infrared camera. Transient pyrolysis outgassing rates have been tracked with spectrometers targeting hydrocarbon molecules in the boundary layer. Virgin and tested samples haven been studied at VKI and in collaboration with EPFL with microscopic and material analysis tools. Simulations of the experiments with material response codes is ongoing. Future experiments in the Plasmatron will target the radiative boundary layer by observing the stagnation line from an on-board spectrometer prepared in collaboration with EM2C of CentraleSupelec.

Keywords: charring ablator, pyrolysis blowing, surface ablation

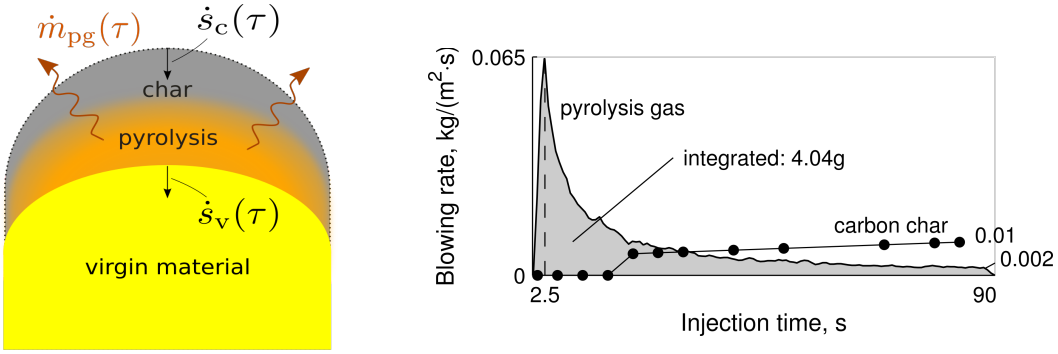

Figure 1: Simplified schematic of mass losses on pyrolyzing ablator (left): transient pyrolysis gas mass loss inside the material leading to consumption of virgin material and char layer removal by recession; including quantitative analysis from experiments for code validation (right). (Images taken from Ref. [2]).

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Ultra-High Temperature Ceramic Coated Carbon-Carbon Composites for Hypersonics

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THERMAL AND MECHANICAL CHARACTERIZATION OF SILICA CLOTH REINFORCED BENZOXAZINE (SCB) COMPOSITES UP TO 2500 °F

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ABSTRACT

Phenolic resole type resins are thermosetting resins that cure through condensation reactions liberating water. If these resins are cured under adequate pressure, the water generated from the condensation reaction is forced into solution and not allowed to exceed its vapor pressure, forming voids. While the process can be utilized to generate a void free composite, water in the free volume of the matrix plasticizes the network and can lead to lower mechanical and thermal performance. As an alternative to traditional phenolic resole type matrix resins, benzoxazine based resins can be used to provide similar molecular structure but do not cure through condensation reactions. Unique features of benzoxazine resins are that matrices containing these materials can be made to have very high thermal stability and char yield. Furthermore, these resins have near zero cure shrinkage and low coefficient of thermal expansion (CTE) when compared to aerospace epoxy matrices. Four variants of a benzoxazine resin based composite were fabricated by Tencate for AMRDEC. Silica fabric (8HS) was used as the fabric reinforcement for each variant. The four variants were 20 and 30% resin content with and without silica filler. Three of these variants were screened for downselection. The testing consisted of mechanical and thermal tests appropriate to evaluate the variants developed as an SRM ablative. This effort will discuss the data from the screening effort and the downselected material. In the screening effort, the following tests were conducted. Thermal tests consisted of thermal expansion through pyrolysis and up to the maximum temperature for the in-situ char at 2500 °F. This was followed up with furnace char experiments to examine the char vs. traditional carbon cloth phenolic (CCP). Remaining thermal tests included conductivity and TGA. Mechanical tests consisted of tension in the fill and across-ply orientations at RT and select elevated temperatures. LHMEL tests and restrained thermal growth (RTG) were also conducted. The test matrix for the downselected material was extensive and comparable to a level I/II matrix.

Review: Development of Type 3 Ablator Response Model under the ESM project

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The process and background for building the roadmap towards Type 3 models for the phenolic impregnated carbon ablator (PICA) is reviewed and summarized. We start with observations from MEDLI (MSL Entry Descent and Landing Instrument) data and SEM (Scanning Electron Microscope) images of core samples from the Stardust flight data, and build the case for a Type 3 model. The requirements for building a Type 3 model are then summarized with place holder models for each component required to build a Type 3 model. Efforts in academia supported under NASA's STMD Early Stage Innovations (ESI) funding are then summarized and placed within the requirements for a comprehensive model. The efforts in developing PuMA (Porous Materials Analysis) codes for computing properties of porous materials from micro-CT (micro-Computer Tomography) images are presented. Finally, a Type 3 model implemented in PATO (Porous-material Analysis Toolbox) is discussed, and some examples of ablative material response using the code are presented.

Orion Multi-Purpose Crew Vehicle (MPCV) Heat Shield: Background Information

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Challenges and Progress towards Reconstruction of EFT-1 Heatshield Aerothermal Environments

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Avcoat versus radiation: potential in-depth absorption and impact on flight instrumentation

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Abstract

Placeholder: The abstract has not made it through our approval system yet.
It should include experimental measurements, radiation transport properties discussion and analysis, and effects on instrumentation.

Keywords: Avcoat, Heat Transfer, Radiation Transport, Flight Instrumentation

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Bridging Micro-Scale and Continuum Material Models for AVCOAT-Like TPS

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Molecular Simulation of Boundary Layer Flow over Thermal Protection System Microstructure

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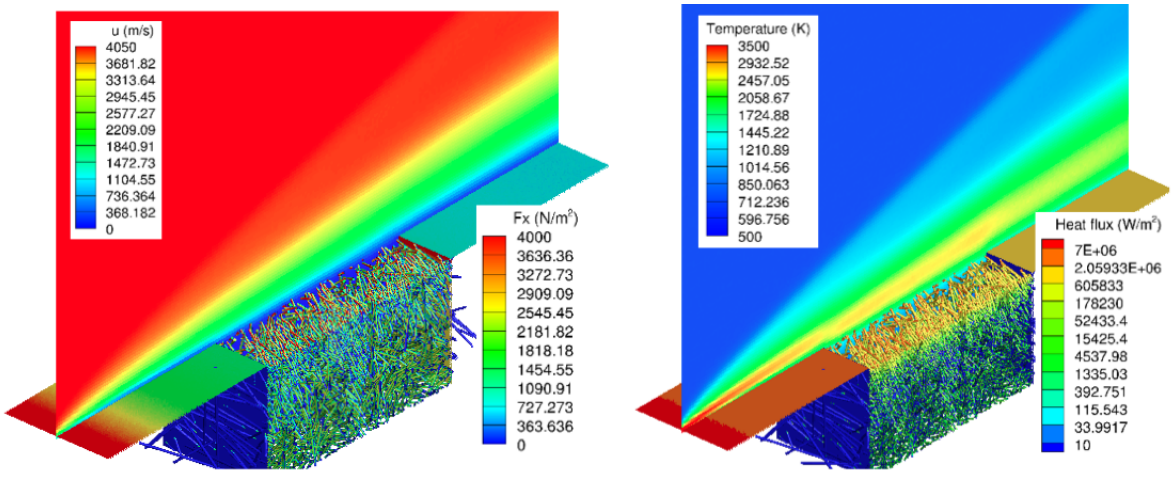
Abstract

Thermal protection systems (TPS) often use ablative materials in scenarios where extremely high heat loads are experienced. The microstructure of the material may influence the overall gas-surface interaction, especially for porous ablative TPS. Furthermore, the flow within the porous material may be locally rarefied. Owing to its non-continuum nature, direct simulation Monte Carlo (DSMC) is a suitable modeling technique for these high temperature rarefied flows.

Based on the results of molecular beam experiments, a finite rate oxidation model has been developed by Poovathingal *et al.* [1]. Surface reaction probabilities, as a function of gas surface temperature, can be obtained from the finite-rate model and used within DSMC simulations. The cut-cell capability in the Molecular Gas Dynamics Simulator (MGDS) code developed at University of Minnesota [2, 3, 4] enables the simulation of flow over the cracks, crevices and protruding granules of realistic TPS microstructures. In addition, x-ray microtomography enables 3D reconstruction of real TPS samples and hence DSMC simulations can be performed on resolved microstructures [5].

Many of the porous ablative materials used for spacecraft TPS are fibrous in nature, embedded within a phenolic resin material that is designed to pyrolyze. Figure 1 shows a DSMC simulation of boundary layer flow over such a porous microstructure. Such simulations can include finite rate carbon-air gas-phase chemistry, gas-surface reactions based on molecular beam experiments, local surface temperature variations in-depth, and even blowing pyrolysis gas. As seen in Fig. 1, the heat flux, shear stresses, and atomic oxygen flux can be determined simultaneously on the microstructure features. The present work will present a parameter study to determine the relative importance of various flow properties on the microstructure.



(a) Shear stress with velocity contour

(b) Heat flux with temperature contour

Figure 1: Heat flux and shear stress on the microstructure

Keywords: Thermal Protection System, Fiber Microstructure, Ablation, Heat Transfer

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In Situ Studies of Ablation Product Yields from PICA and FiberForm Reactions with Molecular Oxygen

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Abstract

The thermal decomposition of phenolic impregnated carbon ablator (PICA) has been investigated with the objective of measuring molar yields of pyrolysis products at heating rates that are relevant to MSL flight conditions. Specifically, PICA has been pyrolyzed at heating rates of 3.1, 6.1, 12.7 and 25 °C s^{-1}, with sample temperatures that spanned a range of 100-1200 °C. Samples were restively heated in a differentially pumped vacuum chamber and pyrolysis gases were measured with a carefully calibrated mass spectrometer. The relative molar yields of 14 pyrolysis gases were obtained in conjunction with mass loss measurements. These measurements allowed for the calculation of absolute molar and mass yields as a function of heating rate, as well as the simulation of TGA curves. Pyrolysis product yields change as a function of heating rate, and this behavior has been attributed to two mechanisms that compete during the initial stages of thermal decomposition. The first reaction involves the condensation of hydroxyl functional groups to form carbon-carbon bonds or ether functional groups. The second reaction involves the breakdown of the methylene bridge between phenol moieties to yield phenol and its derivatives. The second decomposition reaction competes more effectively at higher heating rates. Using the same methodology, we have initiated a series of studies of individual gases with carbon fiber preform or char. The experiments are conducted by allowing a gas to pass through the sample and monitoring the products with a mass spectrometer as a function of time and temperature. The poster will focus on the reactions of molecular oxygen with carbon fiber preform, as well as charred PICA, up to 1800 °C.

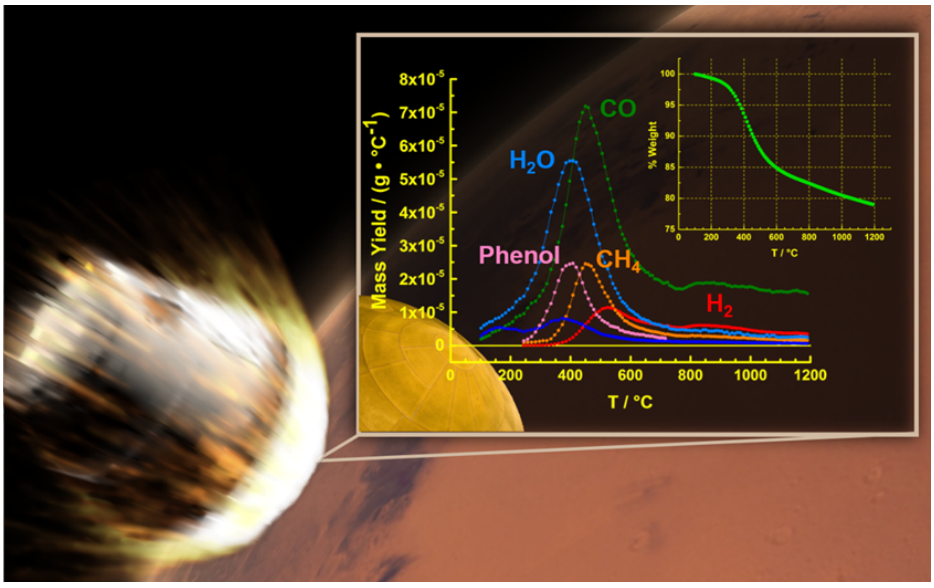

Figure 1: Mass yields of PICA pyrolysis products and simulated TGA at a nominal heating rate of 3.1 °C s^{-1}.

Investigation of the High-Energy Oxidation of FiberForm from DSMC Analysis of Molecular Beam Experiments

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Abstract

In this work, FiberForm®, a carbon preform material used commonly in thermal protection systems (TPS) as a precursor for the Phenolic-Impregnated Carbon Ablator (PICA), is studied computationally using direct simulation Monte Carlo (DSMC). We perform DSMC simulations of molecular beam scattering, replicating experiments of hyperthermal Ar and O/O_2 striking a sample of FiberForm. The detailed micro-structure is obtained from X-ray micro-tomography [1], thus enablisng us to capture the effect of the complex porous and fibrous geometry. The finite-rate surface chemistry model [2, 3] recently constructed from the molecular beam scattering experiments [4] on vitreous carbon was applied to this work, but values of the rate constants were modified slightly to match the experimental data. First, the effect of micro-structure is investigated by studying the non-reactive scattering of argon off the FiberForm sample. A significant portion of the Ar particles were thermally accommodated to the surface temperature, unlike the case of vitreous carbon where all the particles were impulsively scattered. Next, the reactive interaction between the oxygen beam and the FiberForm was investigated. Comparison between the experimental and DSMC time-of-flight (TOF) distributions of both O and CO at 1623 K showed good agreement. Figure 1 shows a comparison between the experimental and numerical TOF distributions, normalized to be able to compare the amplitude of the different peaks. However, it was found that a significantly higher amount of CO was generated when the beam interacted with the FiberForm, when compared with the vitreous carbon. This is postulated to be the a combination of the effects of the differences in the exact micro-structures of the FiberForm sample used in the experiments and simulations, as well as differences in the reactivities of the carbon consituting the two materials studied here.

Keywords: DSMC, surface chemistry, oxidation, gas-surface interaction, ablation.

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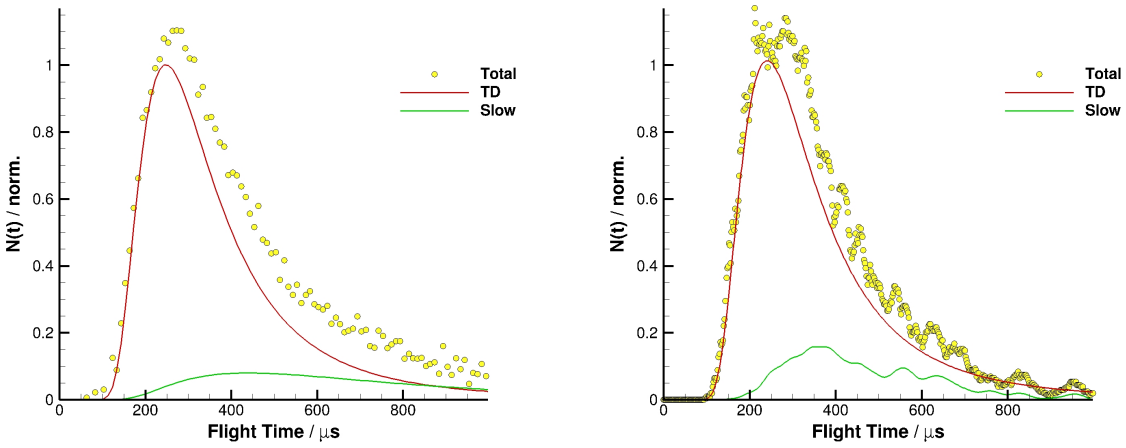

Figure 1: Experimental (left) and numerical (right) normalized TOF distributions of CO molecules scattered from carbon preform surfaces at initial and final angles of 45° at 1623 K.

Modeling of Gas-phase Chemical Kinetics for Pyrolyzing Ablators

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Abstract

Simulations are performed in collaboration with inductively coupled plasma (ICP) torch experiments to validate a gas-phase chemistry model for the boundary layer of a pyrolyzing ablator. A gas injection probe blows CO_2 into a plasma mixture of $Ar/N_2/O_2$, and radiation diagnostics provide measurements of the spectra. A CFD model of the ICP facility [1] is used with a gas-phase finite-rate chemistry model utilizing rates from Martin [2]. Line-of-sight (LOS) spectrum analysis using NEQAIRv14.0 is used to directly compute the radiation spectrum from CFD results, focusing on the CN and Ar lines. Previous work shows good *qualitative* agreement between the experimental and simulated spectra [3]. Recently, developments in the experimental diagnostics provide *absolute* intensity measurements, and allow direct quantitative comparisons between spectra. Excellent agreement is obtained for the case *without* gas injection, but the spectra for various CO_2 blowing rates show a consistent over-prediction of the absolute CN intensity by a factor of 20, and a disagreement in the peak CN location. Future work will focus on improving the agreement between the spectra with CO_2 blowing, and expand the chemistry model to include H_2 injection from the probe.

Keywords: Pyrolysis, Ablation, Gas-phase, Chemistry, Modeling, Validation, Radiation, Spectra

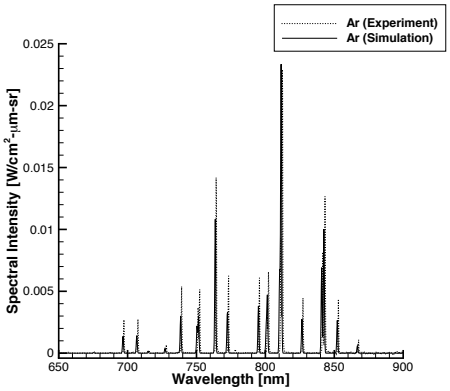

Figure 1: Comparison of Ar spectrum lines for baseline case (without gas injection)

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

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Abstract

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

To quantify and qualify the behavior of the ejected particles, a test campaign was performed at NASA Langley's HYMETS arc-jet facility [1]. In these tests, Fiberform®, AVCOAT, and PICA samples of multiple geometries were subject to various flows. During the experiments, over a three-second interval, high-speed cameras captured images at a sufficiently high rate so that a particular particle could be identified between frames. Using Particle Tracking Velocimetry (PTV), the particle trajectories and kinematic information were developed from the test images. Throughout these experiments, as many as 150,000 trajectories were identified from a single test case.

It is important to know the initial state of the spalled particles to have a better understanding of how the particles are formed, and what process leads to their rapid ejection. To achieve that, initially 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 numerical code that calculates the dynamics of particles [3], developed at the University of Kentucky, is one-way coupled to KATS and then used to determine the initial size, position, and velocity of particles whose trajectories were identified. The preliminary results are presented for the wedge sample.

Keywords: Spallation, Ablation, Arcjet, Thermal protection system

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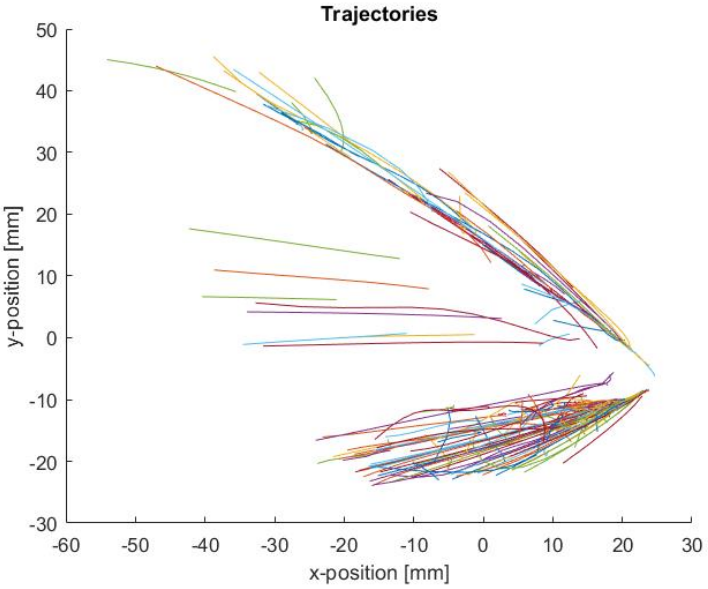
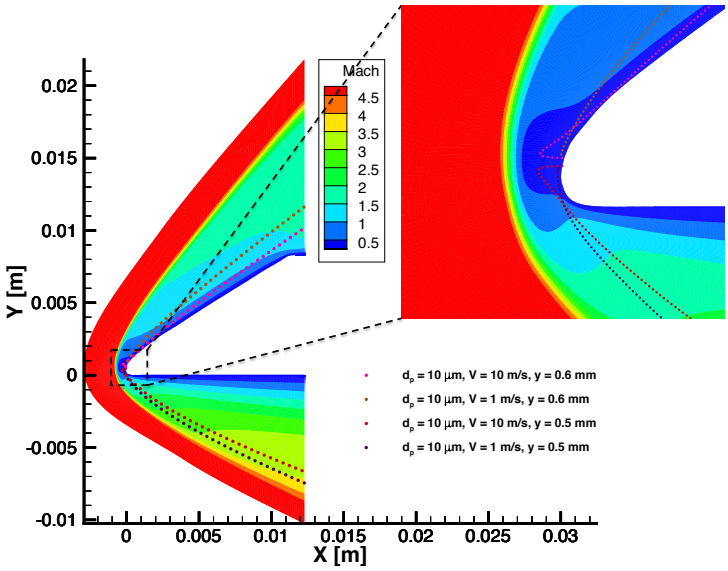
Email addresses: raghava.davuluri@uky.edu (Raghava S. C. Davuluri), james.hardy@uky.edu (James M. Hardy), sean.bailey@uky.edu (Sean C. C. Bailey), alexandre.martin@uky.edu (Alexandre Martin)



(a) Sample of 100 trajectories identified on a Fiberform® wedge sample



(b) Preliminary numerical results based on identified trajectories for a wedge sample

Figure 1: Experimental and Numerical reconstruction of trajectories of particles from a Fiberform® wedge sample

Preliminary Investigation of Ablating Hypersonic Radiating Wake Flows

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and

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[d]*Postdoctoral Researcher, Centre for Hypersonics, The University of Queensland, St Lucia, Queensland, 4072, Australia*
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Abstract

A thermal protection system (TPS) is required for vehicles entering planetary atmospheres to protect crews and payloads from the severe thermal and mechanical loads experienced. Several high-temperature materials have been proposed as possible candidates for hypersonic vehicles including reinforced carbon-carbon and silicon carbide. Despite decades of research, our understanding of the gas-surface interaction of high-temperature materials remains limited. Uncertainties in engineering models used to predict heating and aerodynamics can lead to large factors of safety when determining the thickness of the TPS, which comes at the expense of the mass of the payload available. Much of this uncertainty is due to the inability to accurately predict heating rates, particularly of the afterbody. Though afterbody heating rates are considerably lower than forebody values, uncertainties in the prediction of these values remains significantly higher with radiative heating identified as a major contributor. The uncertainty in predicting afterbody heating is due to the complexity of the flowfield in the wake region. To better understand this complex phenomenon, experiments were conducted at the X2 expansion tunnel at the University of Queensland, Australia. Preheated strips of uncoated carbon-carbon and silicon carbide-coated carbon-carbon were mounted in a two-dimensional compression wedge and tested in 8.5 km/s Earth entry flow. Calibrated spectral measurements were obtained in the expansion region targeting atomic silicon and carbon-nitrogen violet bands for surface temperatures from 1500 K to 2700K. Preliminary results will be discussed and a plan for additional experiments will be presented.

Keywords: Hypersonics, Ablation, Thermal Protection System, Radiation, Wake, Expansion, Carbon-Carbon, Silicon Carbide

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Constructing A New Pyrolysis Model for Carbon/Phenolic Ablators

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Abstract

Accounting for the production of pyrolysis products is an essential step towards developing a realistic model for the response of phenolic impregnated materials used in Thermal Protection Systems (TPS). These models are required to improve margins currently imposed on sizing TPS materials. The objective of this work is to model species generation during the pyrolysis of Phenolic Impregnated Carbon Ablator (PICA) using recently published experimental data. The data used in this study was gathered from Wong et al. [4], Bessire et al. [1], Bessire & Minton [2], and White [5] where TGA data as well as the decomposition products as a function of temperature were carefully measured. An optimization algorithm capable of identifying kinetic parameters from experimental data was developed. The optimization method consists in minimizing the difference between the experimental data on mass loss and simulations based on parallel reaction schemes defined by Arrhenius laws. The space of the kinetic triplet (A, E, n) associated to each reaction is explored based on genetic algorithms (GA) to find the global minimum of the problem. In addition, several heating rates can be used so that a unique set of parameters fit all the data at once. Once the GA has converged, a refinement of the solution is performed using either non-linear least squares or interior-point methods. The model has been implemented and tested in PATO [3], a Type-3 ablation response code. Further development of fitting the pyrolysis experimental data will consider competitive reaction schemes.

Keywords: Phenolic, TGA, Pyrolysis Products, PICA

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Modal Thermal Conductivity Measurement of Fibrous Insulation Materials using a Comparative Cut-Bar Apparatus

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Abstract

A system was developed to measure the effective thermal conductivity of fibrous insulation materials using steady state thermal resistance measurements obtained with a molybdenum comparative cut-bar. By measuring multiple samples with varying thicknesses, the contribution of contact resistance between the sample and the system can be extracted, allowing the the effective thermal conductivity of the sample material to be determined. The modal contribtions of solid conduction between the fibers, gaseous conduction through the gas in the pores, and radiative heat transfer across the pores are isolated by conducting the measurements in environments that selectivley increase or decrease the contribtions of each mode. Conducting measurements in a vacuum to reduce the contribution of gaseous conduction and at low temperatures to reduce the contribution of radiation allows the isolation of solid conduction. With knowedge of the solid conduction contribution, selectively raising the pressure and temperature allows for the isolation of the effective gaseous conductivity and radiative conductivity. Baseline testing was conducted on FiberForm® samples in a 400 K air environment at atmospheric pressure and at 0.15 torr.

Keywords: Effective Thermal Conductivity, Modal Thermal Conductivity, Fibrous Insulation Materials, Comparative Cut-Bar, Heat Transfer

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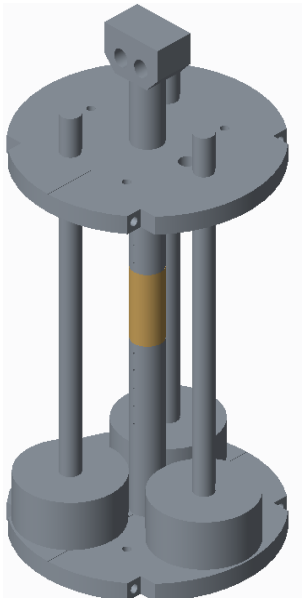
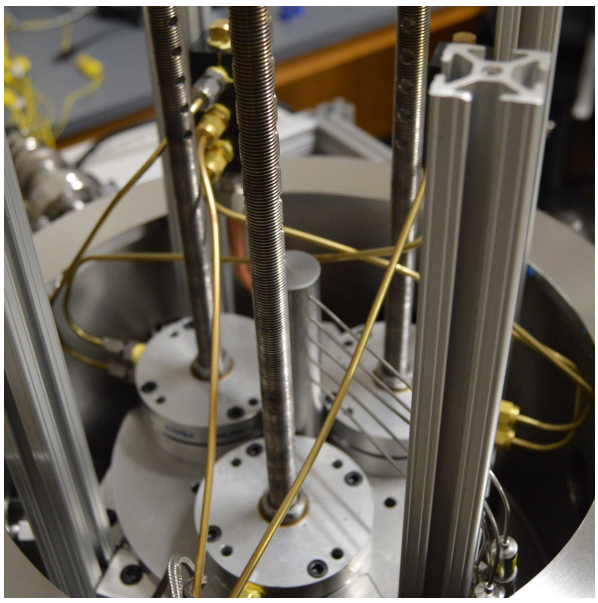
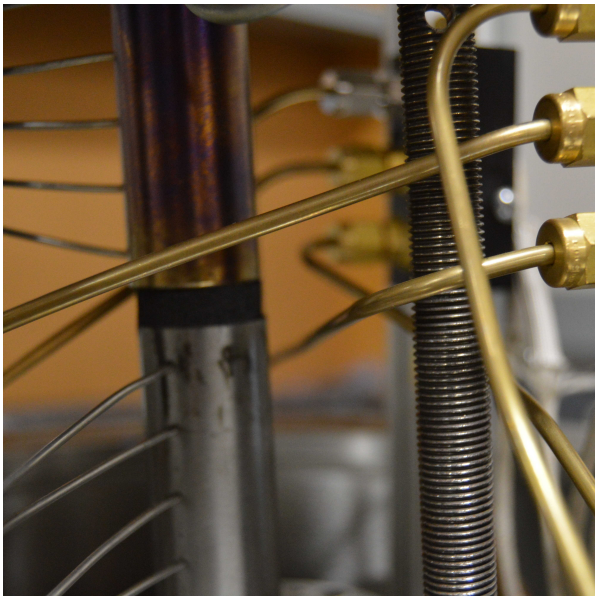


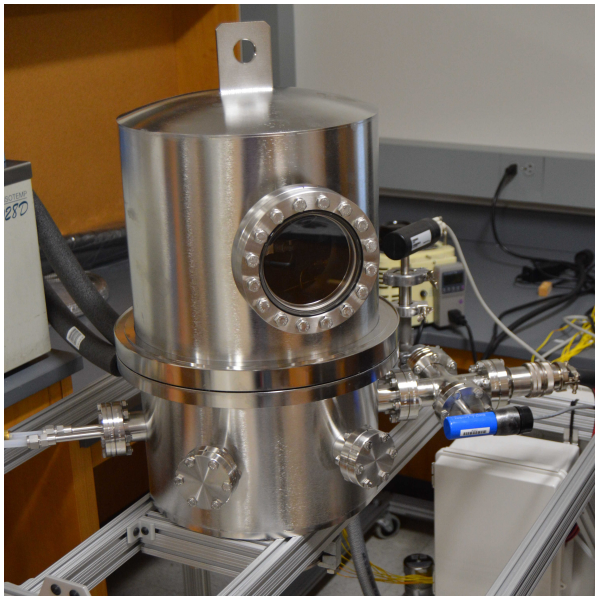
(a) isometric view



(b) bottom cut-bar



(c) sample loaded in cut-bar



(d) vacuum system

Figure 1: Comparative cut-bar thermal conductivity measurement system

Reduction/oxidation experiments on fibrous carbon

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Abstract

Laboratory experiments were carried out to study the decomposition of carbon fibers at high temperature under controlled conditions. Using a furnace heated flow-tube reactor, porous plugs were exposed to controlled rates of O_2, CO2, CO, NO, N and O at temperature between 500 and 1500 K and pressure between 2000 and 6200 Pa. Quantitative measurements of decomposition products were obtained using calibrated mass spectrometry and posttest characterizations of the material samples.

Keywords: Oxidation, Reduction, Ablation , Thermal protection system, Porous media

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DYNAMICS OF GRAPHITE OXIDATION AT HIGH TEMPERATURES

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Gas-surface interactions at high temperatures are of great importance to atmospheric re-entry of spacecraft. Hypersonic flows generate the most extreme thermal conditions experienced by any flight vehicle. For a flight vehicle to survive in this environment, it requires a thermal protection system (TPS) composed of materials that can function at extreme temperatures under harsh oxidizing conditions. Most TPS materials are based on carbon, either in pure form or in a composite. During atmospheric re-entry, these materials are exposed to partially oxidized air at temperatures that can exceed 2000 K. The fundamental reactive and non-reactive dynamics between carbon and atomic or molecular oxygen strongly impact the thermal load on these TPS materials, but they have not been studied in extreme environments such as re-entry.

Hyperthermal interactions of ground-state atomic and molecular oxygen, $O(^3P)$ and O_2 ($^3\Sigma_g^-$) , from a highly oriented pyrolytic carbon (HOPG) surface were investigated with a broad range of surface temperatures from 1100 K to approximately 2300 K. A molecular beam composed of 93% O atoms and 7% O_2, with average translational energies of 5 eV and 10 eV, respectively, was directed at the surface. Translational energy and angular distributions for an incidence angle of $\theta_i = 45°$ were obtained for inelastically and reactively scattered products using a rotatable mass spectrometer detector. Four scattered products were observed: O_2, O, CO and CO_2. The O_2 was attributed to inelastic scattering of O_2 present in the incident molecular beam. Inelastically scattered O atoms exhibited both direct (non-thermal) and indirect (thermal) components. The primary reaction product observed was carbon monoxide (CO); carbon dioxide (CO_2) was observed only with relatively low temperatures. Both reaction products were formed through non-thermal and thermal mechanisms. While there is evidence for direct Eley-Rideal reactions, CO and CO_2 were formed predominantly through thermal reaction mechanisms. The angular flux distributions were peaked about the surface normal and were significantly narrower than a cosine distribution. Additionally, the energies of the desorbing products were much higher than $2RT$ at final angles close to the surface normal and decreased at grazing final angles. Both of these observations indicate that CO and CO_2 are desorbing over a barrier. The components of the non-thermal and thermal CO_2 reactions could not be easily separated in the TOF and angular flux distributions, and a desorption barrier could not be determined for the thermal reaction. The desorption barrier of CO was determined by using the principle of detailed balance. As the surface temperature increased, the amount of CO and CO_2 produced via a thermal mechanism decreased and the calculated desorption barrier for CO increased. Simultaneously, the number of O atoms that scattered via thermal desorption increased, which reduced the number of O atoms available for reaction at higher temperatures. The thermal O atoms were also found to desorb over a barrier which decreased with increasing surface temperature. It is likely that reducing the surface coverage of O atoms caused the desorption barriers for CO and CO_2 to increase. The combined effect of reduced surface coverage and increased desorption barriers apparently limits the reactivity of the surface at extreme temperatures.

Development of VISTA, an open-source Avcoat material model

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Abstract

The re-emergence of Avcoat, used on NASA's current Multi-Purpose Crew Vehicle, has brought the need to reassess properties and engineering performance of the material. In order to further understand the phenomenological physics of the material, an open-source material database has been developed. The present document assembles historical data available from literature to develop a theoretical framework for modeling purposes with the intent of providing a reference standard to the material response community. This proposed material model, dubbed VISTA, allows for direct comparison between codes while allowing for further investigation of Avcoat specific behaviors. The selection process of the properties is presented along with a preliminary assessment of the database performance using historical Apollo thermocouple data.

Keywords: Material Model, Avcoat, TPS

References

*Corresponding author.

Solid Rocket Motor Nozzle Erosion Modeling using Finite-Rate and Equilibrium Methods

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As the first step of the current numerical study, steady-state and unsteady analysis of solid rocket motor (SRM) nozzle throat erosion is performed using commercial code ANSYS Fluent with finite-rate assumption. Both the solid and the fluid regions are modeled as axisymmetric. Heterogeneous finite-rate oxidation reactions [1] are solved on the eroding wall. Multispecies transport equations are included in the analysis and the flow is assumed to be single phase. Erosion rate results of the numerical model are validated using the results from the literature [2] for carbon-carbon throat material and propellants with various aluminum contents. Then, numerical model is implemented to the nozzles of different types of rocket motors of ROKETSAN and results are compared with the post firing measurements.

As well as the numerical studies with the commercial code, a fast decoupled in-house ablation modeling code with equilibrium assumption is also developed for preliminary analysis of SRM throats. The wall properties of an Euler equations solution is assumed to be the boundary layer (B/L) edge properties, and the species concentrations of the flow are not affected by the ablation products. Energy and mass balance are implemented between B/L edge and the wall and the erosion phenomena is assumed to be diffusion-controlled. Equilibrium surface species concentrations are interpolated from readily-prepared equilibrium tables for each calculation iteration. The heat conduction calculation inside the eroding material is obtained with an axisymmetric, anisotropic finite volume code. Effect of recession in the solid region is included using an advection term in the radial direction [3]. The erosion analysis results of the in-house code showed that, successful erosion rate results can be obtained for relatively high wall temperatures and the calculations can be considered as limiting values for mixed diffusion and chemical kinetics controlled erosion cases.

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Thermal Response Analysis of Meteorite Arcjet Experiments Using the Icarus Code

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Abstract

Icarus is a 3-D unstructured material response code[1] under development at NASA Ames Research Center. The Icarus code is intended to be a flexible, efficient, three-dimensional tool capable of simulating the complex thermal protection system (TPS) materials and geometries found in current and future entry architectures. Using modern code development best practices and open source libraries, high-fidelity models for physical phenomenon such as ablation, thermal decomposition, melting, and finite-rate surface chemistry can be easily incorporated into the code.

Arcjet facilities are used to simulate spacecraft environments experienced during atmospheric entry and to test candidate thermal protection system (TPS) materials and systems[2]. Arcjet tests are used in conjunction with computational fluid dynamic (CFD) and in-depth thermal response codes such as Icarus to develop surface recession models for ablating and/or pyrolyzing materials. These computational models, typically based on ground-based (e.g. arcjet) experimental data, are then applied to flight conditions to design and size the TPS on flight vehicles.

In October 2016, an arcjet test was performed in the NASA Ames IHF arcjet facility (designated IHF-317) over a conical test article made from meteorite material as part of the Asteroid Threat Assessment Program (ATAP) to inform models for meteorite ablation. In this presentation, the Icarus material response code will be used to simulate the in-depth thermal response of the IHF-317 test article.

The IHF-317 test conditions were designed to produce stagnation point heating rate and pressure of 4000 W/cm2 and 135 kPa respectively. The total mass flow rate of air and argon was 0.849 kg/s. The average pressure inside the arc heater was 824 kPa, and the bulk enthalpy was 2.14×10^7 J/kg. The DPLR CFD code[3] was used to simulate the flow inside the IHF 6-inch nozzle and around the meteorite test article. Surface film coefficients, enthalpies, and pressures from the CFD solution were used as part of the surface energy balance (SEB) boundary condition for the Icarus simulation. An initial Icarus solution was generated using quartz (SiO2) as the test article material. Temperature contours are shown in Fig. 1. Future work will incorporate newly acquired high-temperature thermal properties for the meteorite specimen into the Icarus material database, and these properties will be used in the Icarus simulation.

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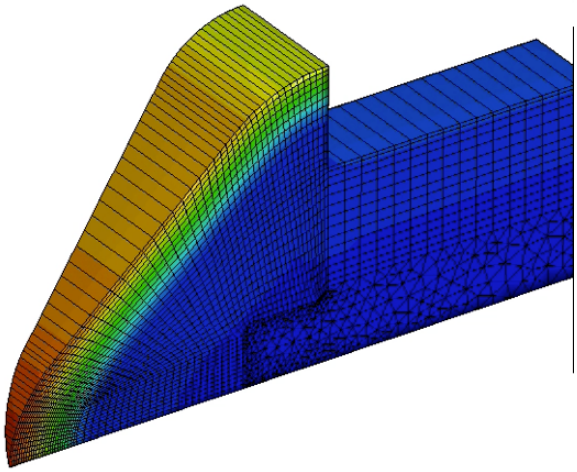

Figure 1: Temperature contours for the meteorite arc jet article.

Flow-tube reactor experiments on the high temperature oxidation of carbon weaves

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Abstract

New generation thermal protection systems (TPS) for exploration entry probes use woven carbon cloths as their main constituting material. Carbon weaves combine superior thermo-mechanical performance to the possibility of tailoring the material micro-structure to certain mission requirements. An application example is the NASA Adaptive Deployable Entry and Placement Technology (ADEPT), a mechanically deployable decelerator, that uses a 3D woven carbon fabric as heat shield material and primary structure.

Under entry conditions carbon weaves decompose via high temperature oxidation. Modeling this phenomenon is a challenging exercise due to the different regimes occurring over a flight trajectory. Current modeling approaches using equilibrium chemistry lead to over-estimated mass loss and material recession. Concurrently, there is a shortcoming of experimental data on the oxidation of ADEPT-like woven carbon fibers that could be used to develop accurate finite-rate chemistry models for ablator response simulations.

In this work, a furnace-heated flow-tube test facility, similar to that developed in previous studies [1, 2], is utilized to measure the surface oxidation of carbon weaves at high temperatures (up to 1600 K) and low pressures (~1000 Pa). Diagnostic equipment is used to monitor temperatures, pressures, and mass flow rate. Real-time analysis of the chemical evolution of oxidation products (CO and CO_2) is collected using a residual gas analyzer mass spectrometer and quantified using calibration experiments with neat gases. Material decomposition products are compared to mass loss measurements on the test samples. We discuss recent progress on experiments under molecular oxygen and carbon dioxide flows and present perspectives in quantifying O-atom oxidation using micro-wave generation and combination of laser-induced fluorescence and gas titration.

Keywords: Woven heat shield materials, oxidation.

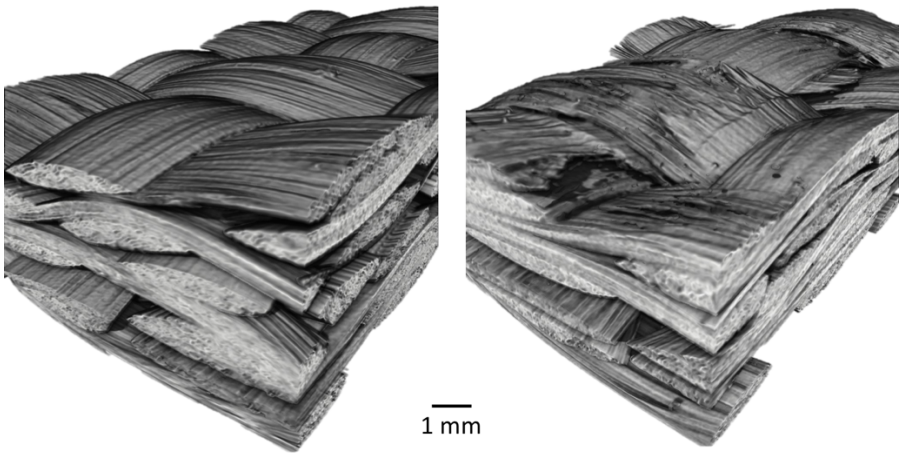

Figure 1: Virgin (left) and ablated (right) carbon fibers

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Scattering Dynamics of Hyperthermal O and O_2 on a Carbon Fiber Network

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Abstract

FiberForm® (FiberForm) is a three-dimensional network of micron-size carbon fibers that is used in ablative heat shields, most notably Phenolic Impregnated Carbon Ablator (PICA). Such heat shields are used in the extreme environments of atmospheric entry, where carbonaceous material is subjected to oxidation by atomic and molecular oxygen at temperatures that range from hundreds to a few thousands of degrees Celsius. We have studied the high-temperature oxidation reactions of FiberForm using a beam of hyperthermal O/O_2 with a mole ratio of $O:O_2$ = 0.92:0.08, where the main oxidation products and different reaction mechanisms were identified from time-of-flight (TOF) and angular distributions. This work follows a similar study in our laboratory on the oxidation of hot vitreous carbon [1]. Aside from the multiple-bounce dynamics that were peculiar to the three-dimensional FiberForm structure, the scattering dynamics of O and O_2 on FiberForm were qualitatively similar to those on vitreous carbon. O_2 was essentially not reactive and scattered through direct scattering and thermal desorption mechanisms. There was significant thermal desorption of O, which increased with temperature. The dominant reactive product was CO, and CO_2 was a minor product; both these products exhibited TOF distributions characteristic of thermal desorption. The flux of the CO product increased with temperature and reached a maximum. Thermal CO products were observed to exit the sample promptly or after relatively long residence times. Two populations of CO with long residence times were distinguished. The results from the FiberForm study suggest that similar reaction mechanisms are occurring on both FiberForm and vitreous carbon and the minor differences observed arise from the three-dimensional porous nature of FiberForm and not chemical reactivity.

Keywords: Molecular beam, atomic oxygen, carbon oxidation

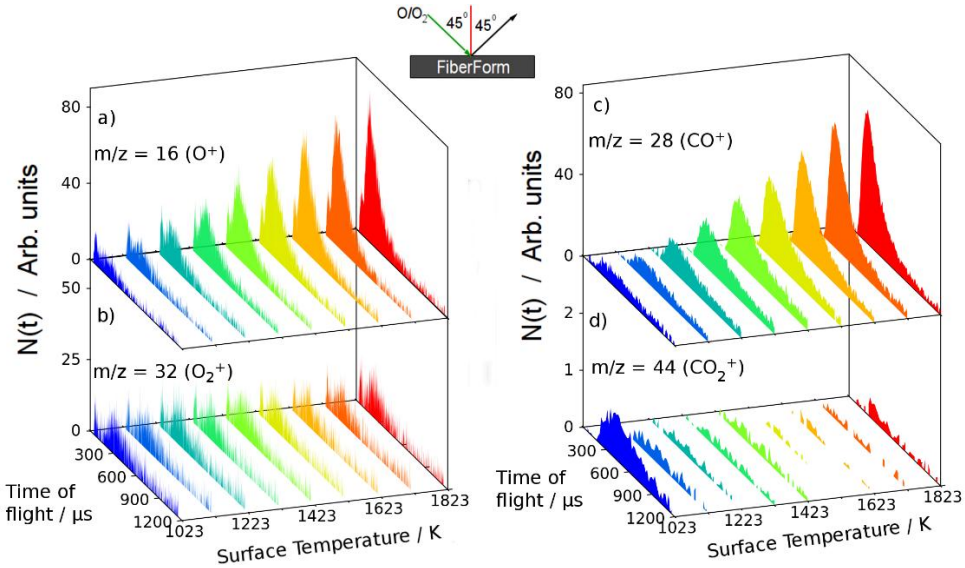

Figure 1: Time-of-flight distributions of O, O_2, CO, and CO_2 with incident O/O_2.

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Hybrid walker approach to conduction-radiation coupling in micro-scale ablation modeling

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Abstract

A high fidelity, multi-scale thermal response model for a multi-phase syntactic foam used in Thermal Protection System (TPS) materials is presented. A complex, micron scale morphology composed of phenolic microballoons and silica fibers is modeled to represent a structure similar to Avcoat TPS [1]. A hybrid CPU-GPU Direct Simulation Monte Carlo (DSMC) solver, CHAOS, [2] is used to model the boundary layer flow through the porous structure. Heat fluxes obtained from the DSMC solver are used as an input to the thermal response solver to simulate heat transfer mechanisms. Based on our previous detailed study of the time scales involved in the flow and thermal response, this process was simulated in a loosely coupled, iterative fashion [1]. In the present work, insights are drawn from a one dimensional (1-D) thermal reponse study conducted to understand the effects of different heat transfer mechanisms on a finite scale material. From this study, the pyrolysis gas blowing rate is obtained at different heat flux loads, which will be used to introduce particles having a directed Maxwellian distribution opposing the incoming boundary layer flow. This will help us understand the interaction of pyrolysis gases with the boundary layer flow and its effect on the thermal response at micron scales.

In the previous work, only the convective heat transfer mechanism was simulated. However, the effects of conduction and radiation can be equally important. In this presentation, we incorporate these effects through a hybrid walker method [3]. To transport heat through conduction and radiation, enthalpy carriers, known as walkers, move about randomly in the domain. This method has been successfully benchmarked for a 1-D heat conduction problem in a rod and the analysis has been extended to simulate conduction on a sphere [4] with different heat flux loads, and a coupled conduction-radiation process between parallel plates. These test cases, which are representative of the underlying problem of heat transfer in phenolic microballoons, serve as a way for detailed verification of the method before it will be coupled with the lumped solver during the thermal response stage.

The culmination of these studies will involve a series of DSMC and thermal response simulations characterized by convection, conduction, and radiation to understand the thermal profile through the material.

Keywords: Heat Transfer, Conduction-Radiation Coupling, Hybrid Random Walker Method

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Verification Studies for the Icarus Material Response Code

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Abstract

Due to the complex physics encountered during re-entry, material response solvers are used for two main purposes: improve the understanding of the physical phenomena; and design and size thermal protection systems (TPS). Icarus [1] is a three-dimensional, unstructured material response tool that is intended to be used for design while maintaining the flexibility to easily implement physical models as needed. Because TPS selection and sizing is critical, it is of the utmost importance that the design tools be extensively verified and validated before their use. The current work aims at partially accomplishing the aforementioned by testing specific functionalities of the code.

A set of verification tests is constructed which aims at insuring that the numerical schemes and equations are implemented correctly through comparison to analytical solutions, grid convergence tests, and code-to-code comparisons. Analytical solutions can provide verification for various types of boundary conditions i.e. transient conduction (Fig. 2), convective heating, radiation, and steady-state ablation. These insure that the physical models and numerics are implemented correctly. Analytical solutions exist for problems of varying geometric complexity, i.e. one-dimensional slabs, two-dimensional cylinders (Fig. 3), and two-dimensional axisymmetric spheres. Performing tests against these solutions insures that grid metrics are consistent with their respective grid element types, and verifies the multi-dimensionality and surface curvature capabilities. Grid convergence tests can be used to insure the order of accuracy is achieved (Fig. 1). Finally, for problems which do not have a known analytical solution, such as thermochemical ablation, comparisons to well-validated codes with comparable physical models can provide confidence that that the fully integrated model is properly implemented. To this end, comparisons with mature material response solvers, such as FIAT[2], CHAR[3], and KATS[4] are presented.

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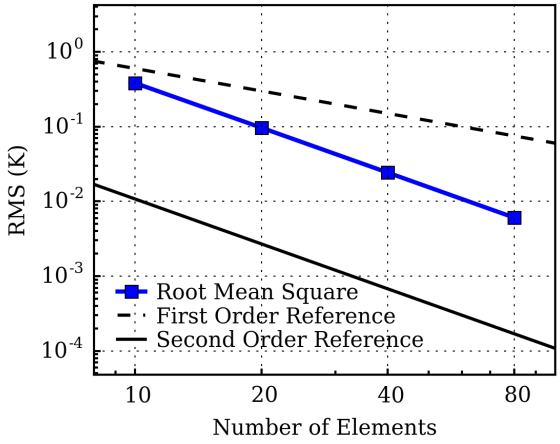

Figure 1: Grid Convergence Test for Transient Conduction with Temperature Dependent Thermal Properties

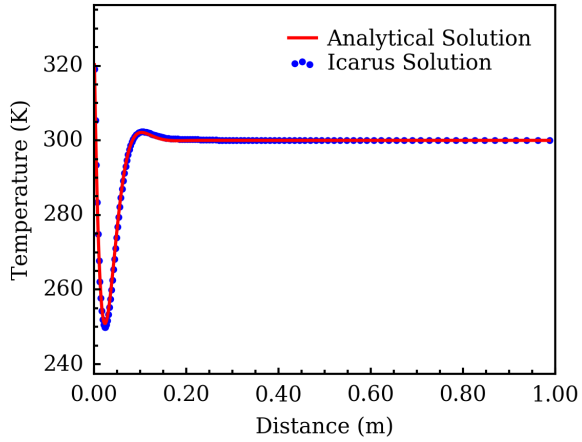

Figure 2: Time-varying Sinusoidal Heat Flux Boundary Condition

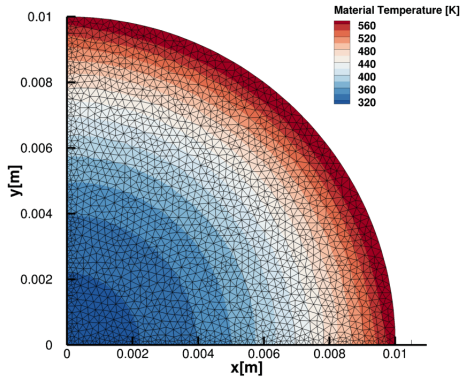

Figure 3: Numerical Solution to a Convective Boundary Condition on a Cylinder

Development of implicit time integration schemes for material response using Icarus

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Abstract

Icarus is an unstructured, three-dimensional finite-volume material response code in active development at NASA Ames Research Center [1]. As a design tool for thermal protection systems (TPS), Icarus uses modern programming practices to allow for the incorporation of various physical models and numerical methods. Previous verification efforts [1] focused on demonstrating the modeling capability for the thermal response of a single material test article using an explicit time integration scheme. While this does much to evaluate the baseline capability of Icarus, it did not address the use of Icarus for practical applications where the thermal response is usually required for long times and explicit time integration schemes are infeasible. The paper focus of this work is on the numerical formulation, implementation, and verification of an implicit time integration scheme for material response modeling in Icarus.

For an implicit time integration method, the flux and source terms are evaluated at the time step, t_{n+1}, which is represented as $\mathbf{F}_{\mathrm{j}}^{n+1}$ and $\mathbf{S}_{\mathrm{i}}^{n+1}$, respectively. The implicit time integration scheme can then be compactly described by

$$\mathbf{U}_{\mathrm{i}}^{n+1} - \mathbf{U}_{\mathrm{i}}^{n} = -\frac{1}{\mathcal{V}_{\mathrm{i}}} \sum_{\mathrm{j} \in J_{\mathrm{i}}} \left[\mathbf{F}_{\mathrm{j}}^{n+1} \cdot \hat{\mathbf{n}}_{\mathrm{j}} \mathcal{S}_{\mathrm{j}} \right]_{\mathrm{i}} \Delta t + \mathbf{S}_{\mathrm{i}}^{n+1} \Delta t. \tag{1}$$

In order to evaluate each j-th surface flux $\mathbf{F}_{\mathrm{j}}^{n+1}$ at the t_{n+1} time, it is necessary to linearize the flux in time using a Taylor series expansion. It is convenient to consider the flux to be a function of $\mathbf{U}_{\mathrm{i}}^{n}$ and $\nabla \mathbf{U}_{\mathrm{i}}^{n}$. Since the fluxes are evaluated at the face centroids, a discrete function, $\mathcal{D}_{\mathrm{j}\to\mathrm{i}}()$, is needed to transform face-centered definitions to their cell-centered values. The expanded flux is described as

$$\mathbf{F}_{\mathrm{j}}^{n+1} = \mathbf{F}_{\mathrm{j}}^{n} + \frac{\partial \mathbf{F}}{\partial \mathbf{U}_{\mathrm{j}}} \mathcal{D}_{\mathrm{j}\to\mathrm{i}} \left(\delta \mathbf{U}_{\mathrm{j}}^{n+1} \right) + \frac{\partial \mathbf{F}}{\partial \nabla \mathbf{U}_{\mathrm{j}}} \mathcal{D}_{\mathrm{j}\to\mathrm{i}} \left(\nabla \delta \mathbf{U}_{\mathrm{j}}^{n+1} \right), \tag{2}$$

where the Jacobians, $\frac{\partial \mathbf{F}}{\partial \mathbf{U}_{\mathrm{j}}}$ and $\frac{\partial \mathbf{F}}{\partial \nabla \mathbf{U}_{\mathrm{j}}}$, are dependent on the system of equations being modeled. As a test problem for the implicit time integration scheme, an initial Gaussian temperature profile is specified on a domain discretized with a stretched grid. Adiabatic boundary conditions are used at all boundaries, and the simulation is run using the implicit time integration scheme at different CFL numbers, which is then compared to the explicitly time-integrated result. Figure 1 shows a summary of the comparisons. In the final work, further verification test cases and timing studies of the implicit time integration scheme will be presented.

Keywords: Heat Transfer, Mass Transfer, Numerical Methods

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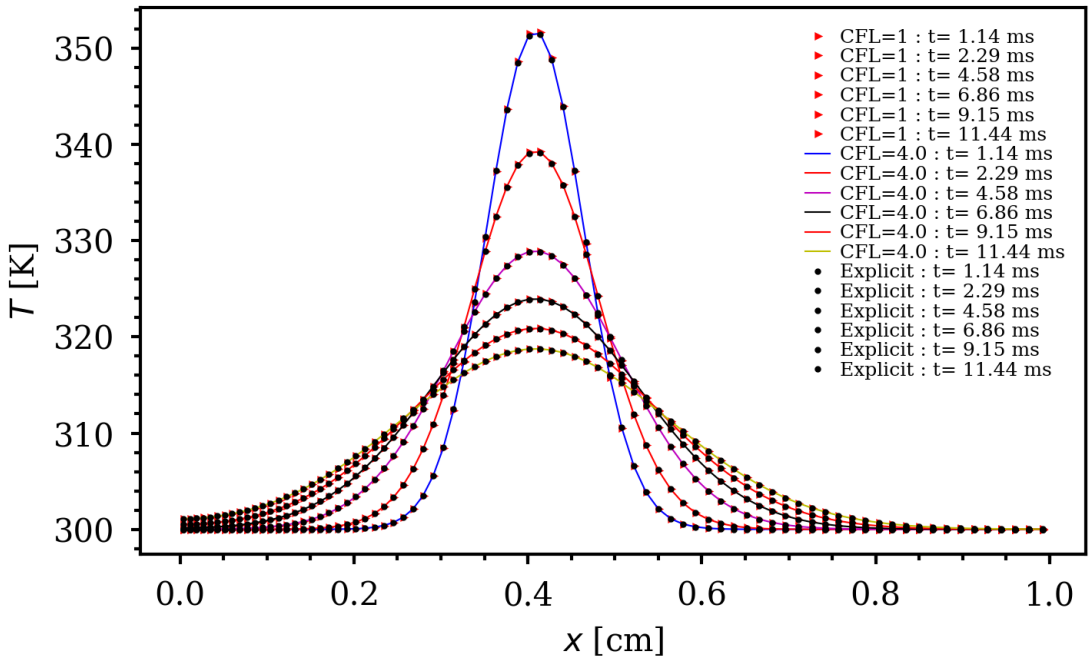

Figure 1: Temperature profiles at different times for an implicit time integration scheme with CFL = 1 and 4 compared to the explicit time integration scheme.

Validation of KATS CFD with Flight Data from KRUPS's KUDOS Launch

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Abstract

Flight data is necessary to validate atmospheric reentry simulations. An ongoing project at the University of Kentucky, the Kentucky Reentry Universal Payload System (KRUPS), has a goal to obtain flight data in an cost effective manner. KUDOS was the first launch of the KRUPS project. This provided temperature reading at various locations throughout the cork TPS. A trajectory code was used to obtain the altitude of maximum heat flux. That heat flux was used as the initial conditions for a flow field simulation that was conducted using the Kentucky Aero-Thermal Solver Computational Fluid Dynamics (KATS CFD). From the CFD solver, the heat flux and edge enthalpy were obtained. The results will be used to model how the material interacts with the environment upon atmospheric reentry using the KATS Material Response (KATS MR) code. Flight data obtained by KRUPS launches will be used to validate KATS CFD and KATS MR for different TPS designs.

Keywords: Computational Fluid Dynamics, Material Response, Atmospheric Reentry,Thermal Protection System, Ablation

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Radiative Heat Transfer Modeling in Fibrous Porous Media

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Abstract

Accounting for radiative heat transfer in porous media is of great significance to sizing materials that meet thermal performance goals of forthcoming space exploration missions. The objective of this work is to compute the effective anisotropic radiative conductivity of fibrous porous media, using highly resolved x-ray tomography images that render a digital representation of the material. An efficient and MPI parallel procedure is developed and verified in comparison to analytical models from the literature for organized and random synthetic fibrous media. Results are then presented for a rigid carbon fiber preform. This material is used to manufacture ablators such as the Phenolic Impregnated Carbon Ablator (PICA), which has been implemented in the thermal protection systems (TPS) of recent successful atmospheric entries. Raw voxel data from the tomographic scans are processed with a Marching Cubes algorithm into a triangulated iso-surface. Relevant view-factors are then obtained using a collision based Monte-Carlo method [1]. The final steady-state heat fluxes into and out of each face are solutions to an algebraic system of coupled equations, with the view-factors as coefficients, which is solved using an under-relaxation iterative method. The radiative conductivity computed is combined with the value calculated for thermal conductivity using *PuMA* [2], a NASA software for extracting porous material properties, to determine the total effective conductivity from the intrinsic conductivity of constituting phases. Results are compared to previous computational studies [3, 4] and to experimental data.

Keywords: Radiative Heat Transfer, Porous Media, Effective Conductivity

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Modeling the Relationship Between Porosity and Permeability During Oxidation of Ablating Materials

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Abstract

Ablative thermal protection systems undergo oxidation when subjected to entry conditions. Decomposition due to oxidation results in an in-depth change in both permeability and porosity. In this study, we focus on the Phenolic Impregnated Carbon Ablator (PICA), a state-of-the-art material used on the Mars Science Laboratory and forthcoming NASA Mars 2020 exploration missions. While the properties of PICA have been extensively studied in recent years, high-fidelity models relating permeability to porosity during oxidation have yet to be developed and validated. To this end, the Porous Material Analysis (PuMA) [1] framework, a software developed by the NASA Ames Research Center, has been used to simulate oxidation based on X-ray tomography images of carbon fibrous materials. PuMA simulates oxidation based on micro-tomography images using a random walk model for diffusion into the porous medium and a sticking probability law for the surface reactions [1]. Analysis was done on FiberForm, the carbon fiber preform of PICA, as well as a low-density felt being considered as the substrate for lightweight conformal carbon/phenolic ablators. Porosity and permeability were both calculated throughout the oxidation process as a function of material decomposition. Based on the computationally oxidized tomographic images, the porosity was determined in PuMA using a thresholding method, and the permeability was calculated using GeoDict [2], a commercial software for calculating porous material properties. A correlation function was then developed to model the relationship between porosity and permeability and compared to analytical correlations from literature for fibrous materials. This model is ideally suited for type-3 ablator response models that take into account the in-depth evolution of the porosity.

Keywords: Porous Media, Permeability, Porosity, Ablation, Oxidation, FiberForm

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KATS-Universal Solver: Validation of Flow Tube Experiments

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Abstract

Modeling the interactions between a porous flow and a plain one, especially for ablating materials, is complex. The conventional approach for analyzing ablation problems includes two parts. On one hand, the high enthalpy flow over the material is simulated with a hypersonic aerothermodynamic computational fluid dynamics (CFD) solver. On the other hand, the mass loss and the temperature change of the material are predicted by a material response (MR) solver. For conjugated ablation problems, the state-of-the-art approach is to use a loosely-coupled method. This method takes the advantages of both the CFD and the MR solvers, but the flow-solid interface is highly simplified. The exchange of information at this interface is increasingly tedious, considering the constant advances in the fidelity of the physical models. Moreover, mesh alignments and movements are not trivial to implement.

As an alternative, a universal solver is a novel idea for approaching conjugated ablation problems, in which both plain and porous flow equations are solved in one system. Using this idea, KATS-Universal Solver (US) is developed based on KATS-MR. The equations and models of KATS-US are verified through analytical problems and benchmark conjugated problems. Moreover, the developed solver is validated through two sets of flow tube experiments. The first set was performed to find the permeability data for argon flow in FiberForm®, using which the permeability model is validated. The second set was performed to study the oxidation behavior of FiberForm® samples. For the highest temperature case (1502K), the major reaction is $C_{(S)} + \frac{1}{2} O_2 \longrightarrow CO$, which is selected as the case and the reaction to validate. The simulation results of solid density profile and gas molar fraction profiles are shown in Figure 1. It illustrates the time history of surface recession of the material and the change of gas species. More importantly, the solver predicts a recession distance and a mass loss within 5% differences to the experiments.

Keywords: Numerical Framework, Porous Media Flow, Validation

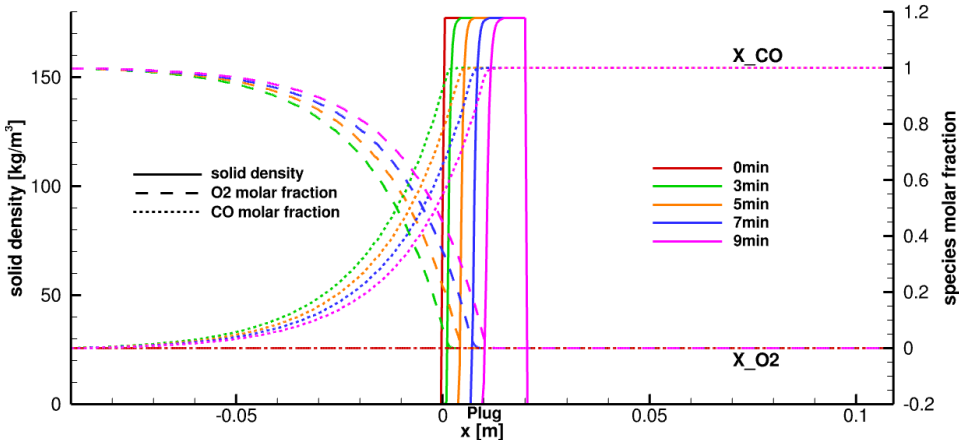

Figure 1: Simulation results of solid density and species molar fractions

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