Doubletree Hotel Albuquerque
201 Marquette Avenue NW | Albuquerque, NM 87102-2248

Agenda Day 1 - March 1, 2011

TIME	TOPIC	SPEAKER
0800-0830	Registration	John Schmisseur, AFOSR Michael Wright, NASA ARC
	Introduction/Overview Chairs: John Schmisseur and Michael Wright	
0830-0840	Introduction	Ioana Cozmuta ERC
0840-0900	ITAR Regulations in AFOSR	Jonathan Griffin AFOSR
0900-0920	Ablator Modeling: Why Not Much has Changed Over the Past 45+ Years?	Bernie Laub NASA ARC
0920-0940	NASA Uncertainties Management in the TPS Design Process	Michael Wright NASA ARC
0940-1000	Phenomena and Material Property Requirements for a Combined Structural and Thermal Ablation Model	Mark Ewing ATK Aerospace Systems
1000-1015	**BREAK**	
1015-1045	Current Activities for Evaluation and Prediction of Ablator TPS Performance at JAXA ARD	Kazuhisa Fujita JAXA
1045-1115	Astrium R&D Approach for TPS Development and Modeling	Jean-Marc Bouilly Astrium
1115-1140	Sandia Perspective on Ablative Material Testing	Justin Smith Sandia
1140-1205	NASA TPS Development for Future EDL Missions	Robin Beck NASA ARC
1205-1330	**LUNCH/POSTER SESSION [See listing at the end of the agenda]**	
	In-Depth Physics and Chemistry of Ablation Chairs: Jean Lachaud and Ioana Cozmuta	
1330-1355	Experimental Data Needed for High-Fidelity Material Response Models	Jean Lachaud University of California-Santa Cruz
1355-1420	Experimental Characterization Methods for Three-Dimensional Microstructure Analysis	Elizabeth Dickey North Carolina State University
1420-1445	Internal Reactions in Porous Carbon Chars – A Flow-Tube Reactor Approach	Jochen Marschall SRI
1445-1510	Challenges Characterizing Ablators Properties: Experimental Techniques and Associated Uncertainties	Jay Feldman ERC
1510-1525	**BREAK**	
1525-1550	Mass Spectrometry of Pyrolysis Products During Thermal Decomposition of Ablator Materials	Jason White SRI
1550-1615	Using FT-IR Spectroscopy to Elucidate the Structures of Ablative Polymers	Wendy Fan ERC

1615-1640	Measurement of Mass Transport Properties of Carbon Phenolic Ablator Materials and Their Relationship to a Material's Behavior in use Environments	Eric Stokes Southern Research Institute
1640-1705	Nitric Oxide PLIF Measurements in the Hypersonic Materials Environmental Test System (HYMETS)	Paul Danehy NASA LaRC
1650-1730	Group Discussion	All
1730	**MEETING ADJOURNED FOR THE DAY**	

Agenda Day 2 - March 2, 2011		
TIME	**TOPIC**	**SPEAKER**
0745-0800	Registration	
Gas Surface Interaction and Catalysis **Chairs: Matthew MacLean and Jochen Marschall**		
0800-0825	Return of Hyabusa Sample Return Capsule and Japanese Ablator Technologies	Tetsuya Yamada JAXA
0825-0850	Investigation of Gas-Surface Interactions of Innovative Carbon Composite Ablators in the 1.2MW VKI Plasmatron	Olivier Chazot VKI
0850-0915	Recent Gas-Surface Interaction Measurements in the 30kW ICP Torch Facility	Douglas Fletcher University of Vermont
0915-0940	High Enthalpy Ablation Testing at DLR	Bunkard Esser German Aerospace
0940-0950	**BREAK**	
0950-1015	GSI Modeling Overview: Requirements for Macroscopic Gas/Surface Interaction Coupling in CFD Codes	Matthew MacLean CUBRC
1015-1040	Surface Catalysis Measurements Using a Diffusion-Tube Side-Arm Reactor	Jochen Marschall SRI
1040-1105	Oxidation Behavior of Ultra-High Temperature Ceramics Using Different High Temperature Test facilities	Erica Corral University of Arizona
1105-1130	Characterizing TPS Microstructure – Review of Some Techniques to Capture and Quantify Scale of Microstructure	Mathew Gasch NASA Ames
1130-1155	In Situ Techniques to Understand Changes in Surface Chemistry During Ablation	Samir Aouadi Southern Illinois University
1155-1220	Atomistic to Macroscopic Modeling and Validation for Gas-Surface Interactions	Tom Schwartzentruber University of Minnesota
1220-1330	**LUNCH/POSTER SESSION [See listing at the end of the agenda]**	
Roughness Modeling with Gas Blowing Effects **Chairs: Adam Amar and Charles Powars**		
1330-1355	Overview of Roughness and Blowing Effects in Flows Over Ablating Surfaces	Charles Powars St. Croix Research
1355-1420	Fundamental Studies of Surface Roughness and Ablating Flows	Rodney Bowersox Texas A&M University
1420-1445	Experimental Investigations of Surface Roughness and Blowing Effects on Heat Transfer in Hypersonic Shock Tunnels	Michael Holden CUBRC
1445-1510	Surface Roughness Characterization and Modeling	Yvan Aspa Astrium
1510-1520	**BREAK**	

1520-1545	A Combined Numerical and Experimental Investigation of the Coupling Mechanisms Between an Ablative Wall and Turbulence	Christopher White University of New Hampshire
1545-1610	Prospects for DNS and LES of Ablating Surfaces	Graham Candler University of Minnesota
1610-1635	Spatially and Temporally Resolved Data of High Enthalpy Turbulent Boundary Layers	Pino Martin University of Maryland
1635-1700	Simulation of Surface Roughness Effects on Hypersonic Blunt Body Reentry Heating	Yehia Rizk NASA ARC
1700-1730	Group Discussion for Gas Surface Interactions and Roughness Modeling Sessions	All
1730	**MEETING ADJOURNED FOR THE DAY**	

Agenda Day 3 - March 3, 2011		
TIME	**TOPIC**	**SPEAKER**
0800-0810	Registration	
0810-0830	Introduction to the NASA Thermal Performance Database	Richard French NASA JPL
Ablation Model Code Intercalibration Exercise Jean Lachaud- Moderator		
0830-0845	Presentation of the Ablation Modeling Intercalibration Test Case	Jean Lachaud UCSC
0845-0855	Presentation of FIAT Baseline Results	Bernie Laub NASA ARC
0855-1005	Intercalibration Results (**5 minutes/participant)**	
	0855-0900 MOPAR — Alexandre Martin (University of Kentucky), Jon Wiebenga, Iain D. Boyd (University of Michigan) 0900-0905 NEQAP — James B. Scoggins and Hassan A. Hassan (NC State University) 0905-0910 PATO — Jean Lachaud (UARC - UCSC) and Nagi N. Mansour (NASA - ARC) 0910-0915 NIDA — Gary C. Cheng and Balaji Shankar Venkatachari (University of Alabama, Birmingham) 0915-0920 US3D Module — Graham Candler (University of Minnesota) 0920-0925 Amaryllis — A.J. van Eekelen (SAMTECH), G. Pinaud, and J.-M. Bouilly (Astrium SAS) 0925-0930 libAblation — Rochan Upadhyay (University of Texas at Austin) 0930-0935 Chaleur — Ben Blackwell, Micah Howard and Dave Kuntz (Sandia) 0935-0940 MIG — Ankush Bhatia and Subrata Roy (University of Florida) 0940-0945 KCMA — Phillipe Reynier (ISA) 0945-0950 CAT — Nagi N. Mansour (NASA ARC), J. Lachaud (UARC - UCSC), T. Magin and J. de Muelenaere (VKI) 0950-0955 CMA — Micah Howard, Dave Kuntz and Ben Blackwell (Sandia) 0955-1000 CHAP — Pete Keller (Boeing) 1000-1005 HERO — Mark E. Ewing and David E. Richardson (ATK)	
1005-1015	Imponderable and Webex call-ins	
1015-1030	Overview of Results	TPDB
1030-1100	**BREAK (Around the Posters)**	

1100-1120	Discussion of Next Round of Intercalibration Test Conditions	Alexandre Martin University of Kentucky
1120-1200	Future Validation Experiments (round table discussion)	Moderator: Jean Marc Bouilly Astrium
1200-1230	Outcome of the Workshop and Future Directions	Ioana Cozmuta ERC Inc
1230	**MEETING ADJOURNED**	

Poster Session Listing Next Pages

POSTER SESSION PESENTATIONS
(Posters will be displayed both days with some left for Thursday)

	Presenter Name	Poster Title
1	**Milad Mahzari** Georgia Tech	An Inverse Parameter Estimation Methodology for the Analysis of Aeroheating and Thermal Protection System Experimental Data
2	**Alexandre Martin** University of Kentucky	Carbon-phenolic-in-air Chemistry model for Atmospheric Re-entry
3	**Erin D. Farbar** University of Michigan	Modeling of Ablation using the DSMC Method
4	**Ofodike Ezekoye** University of Texas - Austin	Extension of the PECOS Quasi-steady Ablation Toolkit for Uncertainty Propagation
5	**Alina Alexeenko** Purdue	Feasibility of Ablation Measurements in Small Particle Hypervelocity Impact Range Facility
6	**Paul Norman** University of Minnesota	Modeling Air-SiO2 Surface Catalysis under Hypersonic Conditions with ReaxFF Molecular Dynamics
7	**David R. Payne** Defense Science and Technology Lab	Experimental Support for Ablation Model Parameter Development
8	**Jose Santos** Sierra Lobo	Catalysis and Oxidation of Copper Calorimeters-Are We Over Testing Material Samples?
9	**Maria Gritsevich** University of Helsinki/ Moscow State University	Ablation and Drag Modeling for Reentry of a Blunt Body with Complex Geometry
10	**E Titov** Penn State	Modeling of Crack Propagation in AVCOAT, a Charring Ablator
11	**Paul M Danehy** NASA Langley	Nitric Oxide PLIF Measurements in the Hypersonic Materials Environmental Test System (HyMETS)
12	**Jean Marc Bouilly** Astrium	Astrium R&D Approach for TPS Development and Modelling
13	**Alexandre Martin** University of Kentucky	MOPAR: Inter-code Calibration of Charring Material Response
14	**Ben Blackwell** SANDIA	Prediction of Density Degradation of Low Density Material Using the CHALEUR Code
15	**Ankush Bhatia** University of Florida	MIG: Results for the Inter-code Calibration Exercise
16	**A.J. van Eekelen** Astrium	AEROFAST: Thermal/Ablation Analysis of the Front Heat Shield for a Martian Aerocapture Mission
17	**Gary Cheng** UAB	NIDA – A Non-Equilibrium based In-Depth Ablation Code
18	**Graham Candler** University of Minnesota	A Conservation Law Form of the CMA In-depth Ablation Model
19	**Mark Ewing** ATK	HERO: Heat Transfer and Erosion Analysis Program
20	**JB Scoggins** NCSU	NEQAP: Nonequilibrium Ablation and Pyrolysis-a Fundamental Approach
21	**Micah Howard** SANDIA	Prediction of Material Decomposition of a Low Density Material Using the CMA Code
22	**Peter Keller** The Boeing Co	CHAP (Convective Heating and Ablation Program)
23	**Jean Lachaud** UARC	PATO Results for the 2011 Ablation Test Case
24	**Nagi N Mansour** NASA ARC	Charring Ablator Thermal Response Model (CAT) -a High-Fidelity Material Response Model

25	**Philippe Reynier** ISA	Numerical Rebuilding of Ablative Test Cases Using KCMA
26	**Rochan R Upadhyay** University of Texas - Austin	Description and Results of a Predictive Model for Pyrolysis: libAblation
27	**Jim Merrifield** Fluid Gravity Engineering Ltd	Computation of the TACOT Intercalibration Test Case for the 4th AFOSR/SNL/NASA Ablation Workshop using FABL
28	**Ryan Gosse** AFRL	Title TBD
29	**Brian Remark** NASA JSC	STAB

IN-DEPTH PHYSICS AND CHEMISTRY OF ABLATION
CHAIRS: JEAN LACHAUD AND IOANA COZMUTA

Structure and Motivation of the 4th non-ITAR Ablator Modeling Workshop

Ioana Cozmuta, ERC. Inc, USA

The 4th edition (2011) of the Ablation Modeling workshop focuses on the experimental support required for the development and validation of high fidelity models in the following areas:

1. In-depth physics and chemistry of ablation
2. Gas-surface interactions and catalysis
3. Roughness modeling including wall-blowing effects
4. Ablation models inter-code calibration and validation
5. Poster session dedicated to various existing modeling efforts

The emphasis for each of the target areas is the material contribution as opposed to the aerothermodynamics. With the workshop being the first non-ITAR edition we are seeking to expose the broader (national and international) community to the particular issues involved with material response modeling under hypersonic reentry conditions in the hopes of bringing new experimental techniques to bear on the problem as well as brainstorm about the challenges faced by expanding the range of application of the existing techniques.

It is also for the first time that we provided the ablation community at large with a test case for a theoretical ablator to compare results of various ablation codes and identify the role of different implementations on the predicted output results.

From the perspective of TPS design, high fidelity models play a critical role since they enable anchoring of engineering codes with better represented physics and chemistry models, ability to perform sensitivity trades and identify major contributors to the overall thickness of the heatshield and lay the path for rational design for ablator materials in support of future missions as well as better use of flight data via inverse parameter estimation techniques.

ITAR Regulations in AFOSR

Lt. Jonathan Griffin, Air Force Office of Scientific Research, USA

An overview of the relevant portions of U.S. export control regulations contained in the International Traffic in Arms Regulation (ITAR) and the Export Administration Regulation (EAR). An emphasis will be placed on discussing how the ITAR applies to basic research conducted at academic institutions

Ablator Modeling: Why Not Much Has Changed Over the Past 45+ Years

Bernard Laub, NASA Ames Research Center, USA

In the late 1950s, the earliest models describing the thermal response of ablative materials were based on the heat of ablation concept, which is an empirical approach that was reasonable for the types of materials of interest at that time. In the early-mid 60s the models were expanded to include pyrolysis since organic resin composites became the TPS materials of interest. However, surface recession was still predominantly modeled via empirical correlation. The development of the 1-D CMA finite difference code in the mid-late 60s introduced the thermochemical ablation approach for gas/surface interactions. Since that time investigators have developed finite volume and finite element codes, in 1-D, 2-D and 3-D, but the basic modeling has not evolved significantly. Models describing internal gas pressure due to pyrolysis, particle impact erosion, in-depth radiant transport, etc., have been added to address specific problems, but the fundamental modeling has not evolved. The reasons for this *stagnation*, as viewed by the author, will be described.

NASA Uncertainties Management in the TPS Design Process

Michael J. Wright, NASA Ames Research Center, USA

The process of designing a thermal protection system for an entry vehicle involves many stages, including selection and sizing of the TPS material, thermal and structural design of the TPS to accommodate mission requirements, and detailed design of the resultant aeroshell to accommodate singularities such as penetrations, windows, attachments, and other engineering requirements. Unlike many spacecraft subsystems, TPS is designed primarily via computational methods, validated with component level ground tests that do not simulate all aspects of the flight environment. The employed physical models are thus used to extrapolate ground test results to the expected flight environment. This ground-to-flight traceability places great emphasis on using high-fidelity models that accurately simulate the necessary underlying physics and chemistry, so that the extrapolation to flight can be performed confidently. This talk will focus on key uncertainties primarily in the first steps of the process, namely the thermal sizing of the TPS material to meet mission requirements and reliability. The TPS sizing process requires a good understanding of the aerothermal environment encountered and the uncertainties in that environment, as well as a good TPS thermal response model that is capable of accurately determining the thickness of material required to maintain an acceptable bondline temperature in the face of the encountered environment. Uncertainties in both the environment encountered and the TPS response to that environment are captured and used to define a thermal margin policy that is tailored to the mission and overall reliability required. While a large amount of literature has been published discussing and defining the impact of aerothermal uncertainties on TPS sizing, much less work has been done to define the impact of material response uncertainties. These uncertainties tend to fall in three major areas: gas-surface interactions (the chemical interaction of the TPS material with the environment), roughness and blowing effects (the fluid dynamic interaction), and in-depth chemistry (the means by which ablating materials accommodate large heat loads efficiently). Examples will be given in each of these areas where our current lack of understanding of the underlying physics can lead to either large design margins and/or low reliability in the final design.

Phenomena and Material Property Requirements for a Combined Structural and Thermal Ablation Model

Mark E. Ewing and David E. Richardson, ATK Aerospace Systems, USA

The primary physical response phenomena associated with ablative insulators are discussed in this presentation. Ablative insulators are typically heated by radiation and convection at an exposed surface. As regions within the insulator increase in temperature the material decomposes (pyrolizes), and a pyrolysis front progresses into the insulator leaving behind a layer of charred material. Pyrolysis gases are generated as the material chars, and these gases flow through and exchange energy with the porous char structure. Meanwhile, erosion of the surface material can occur due to chemical and mechanical interaction with the boundary flow. Thermal modeling approaches used to simulate these phenomena are discussed in this presentation with a focus on the in-depth material response. In addition to thermal modeling, structural modeling is often required for accurate assessment of phenomena such as pocketing, ply-lifting, wedge-outs, and delaminations, all of which can dramatically affect the thermal protection ability of an ablative insulator. Structural material responses are integrally tied to thermal responses. For example, the moduli can be dependent on the degree-of-char, which is integrally tied to the thermal history. In addition, material stiffness and capabilities have been shown to be tied to the amount of moisture present in the material, which is also tied to the thermal response. Structural behavior is also influenced by pressures in the material (calculated with thermal codes), and pressure magnitudes are highly dependent on structural loading (calculated with structural codes). Conjugate models are therefore required for accurate simulation of the thermal and structural behavior of ablative insulators. This presentation outlines areas where this coupling is required and describes associated property requirements.

Current Activities for Evaluation and Prediction of Ablator TPS Performance at JAXA ARD

Kazuhisa Fujita, Japan Aerospace Exploration Agency, Japan

JAXA ARD has been developing a comprehensive test system for experimental evaluation of the ablator TPS performance as well as numerical prediction in flight. To enhance accuracy and reliability of heating tests, the thermochemical state of test flow has been studied so far in detail, and now continuously monitored during heating tests. The SCMA code for ablator analysis has been extended to deal with multi-dimensional problems and to be coupled with test flow analysis, taking into account anisotropy of TPS materials and advanced thermochemical models, such as nonequilibrium oxidation and nitridation. The heating test results are compared with the numerical results so that overall understanding the heating test can be obtained. The above test techniques have been validated using a variety of ablators, and now applied to light-weight ablators under development.

Astrium R&D Approach for TPS Development and Modeling

Jean-Marc Bouilly, Astrium, EADS, Europe

After a reminder of the main general considerations driving TPS development, this talk will present the current R&D project in which this subject is treated. An overview will be given about the scientific or industrial cooperations that are being implemented to address various topics such as material elaboration, material modeling, or related aerothermodynamic aspects.

Sandia Perspective on Ablative Material Testing

Justin Smith and Dave Kuntz, Sandia National Laboratory, USA

Sandia National Laboratories supports DOE missions by designing, building, and flying hypersonic flight vehicles and has over 40 years of experience in these activities. Prior to flight, the development, analysis, and testing of advanced materials in severe environments is often required. This presentation will highlight Sandia's perspective on the development and testing of materials needed to support hypersonic flight vehicles. Included in this presentation will be a discussion of flight environments (including aerodynamic heating, chemistry, and boundary layer transition), thermal protection system (TPS) material development, and ablative and non-ablative material testing. Sandia's experience in testing at ground-based facilities including wind tunnels, radiative facilities, sled tracks, and arc jets will also be presented. Gaps in current test capabilities will be discussed with emphasis on the needs of proposed future flight tests.

Overview of NASA's Current Materials Development Efforts for Mars EDL

Robin Beck, NASA Ames Research Center, USA

Current roadmaps point to landing heavy masses (cargo, followed by manned vehicles) on Mars in the 2030's and the existing entry, descent and landing (EDL) technology will not be sufficient to facilitate such missions. In 2009 the Exploration Technology Development Program (ETDP) established the Entry, Descent and Landing Technology Development Project (EDL TDP), to be managed programmatically at Langley Research Center (LaRC) and technically at Ames Research Center (ARC). The purpose of the project is to further the technologies required to land heavy (~40 metric ton) masses on Mars to facilitate exploration. The EDL TDP contains three technical elements. They are:
1) Thermal Protection Systems (TPS) development
2) Modeling and Tools (MAT) development
3) Supersonic Retropropulsion (SRP) development
The primary goals of the EDL TDP TPS element is to design and develop TPS materials capable of withstanding the severe aerothermal loads associated with aerocapture and entry into the Martian atmosphere while significantly decreasing the TPS mass fraction contribution to the entry system. Significant advancements in TPS materials technology are needed in order to enable heavy mass payloads to be successfully landed on the Martian surface for robotic precursor and subsequent human exploration missions. The EDL TDP TPS element is further divided into two different TPS concepts for Mars EDL those being:

- Rigid TPS for a mid L/D aeroshell with the capability to withstand dual pulsed heating environments as high as 500 W/cm2 for aerocapture and 130 W/cm2 for entry
- Flexible TPS for a deployable aerodynamic decelerator with the capability to withstand dual pulsed heating environments as high as 120 W/cm2 for aerocapture and 30 W/cm2 for entry

NASA, along with its vendors, has begun developing and testing materials for each of the deceleration approaches. These include multi-layer rigid ablators and flexible ablative materials. In order to model the response of these types of materials, new and improved modeling techniques will be required. This presentation will outline the types of materials that are under development and illustrate the need for advancement in modeling of ablative materials.

IN-DEPTH PHYSICS AND CHEMISTRY OF ABLATION
CHAIRS: JEAN LACHAUD AND IOANA COZMUTA

Experimental Data Need for High-Fidelity Material-Response Models

Jean Lachaud (UCSC), Ioana Cozmuta (ERC), Nagi Mansour (NASA Ames)

Objective of the session

Several high-fidelity material-response models are being developed by the hypersonic community. These models require, in addition to the input parameters traditionally used in the state-of-the-art material-response codes, data not currently available - at least in the open literature. The presentations in the session will describe both state-of-the-art experimental techniques and innovative methods in support of model development and data acquisition for high-fidelity models.

In-depth phenomena, high-fidelity models, and required data

As a practical introduction and to provide orders of magnitude, we will describe the in-depth physico-chemical phenomena occurring in a low-density fibrous ablator under conditions relevant to sample return missions. A general high-fidelity model will be presented. The mass, momentum, and energy conservation equations and associated input parameters will be described. The focus will be set on the associated experimental data needed. We will conclude the presentation with a table summarizing the parameters that need to be determined and refer to the contributions of the session that will describe in details specific experimental techniques.

Table of parameters

Symbols (unit)	Properties	Exp. Techniques	Status	Presentations
Conservation of mass				
ε (-)	Open porosity	Pycnometry	SoA	M. Gasch
		Tomography	AM	E. Dickey
$\varepsilon_{mat.}$, ε_{fiber} (kg m^{-3})	Volume fractions	From elaboration	SoA	J. Lachaud
		Tomography, SEM	AD	E. Dickey
$\rho_{mat.}$, ρ_{fiber} (kg m^{-3})	Intrinsic densities	Densitometry	SoA	M. Gasch
		Tomography	AM	E. Dickey
π (kg m^{-3} s^{-1})	Overall Pyrolysis rate	TGA	SoA	J. Feldman
π_i (mol m^{-3} s^{-1})	Pyrolysis rate and species production	TGA + spectrometry	AD	J. White
		FT-IR Spectroscopy	AD	W. Fan
ω_i (mol m^{-3} s^{-1})	Finite-rate chemistry of the pyrolysis gases	Flow-Tube Reactor + spectrometry	AD	J. Marschall
Mass transport				
K (m^2), Fo (-),	Permeability, Forch-	Permeameter	SoA	E. Stokes

β (N)	heimer, Klinkenberg	Tomography + DNS	AM	E. Dickey/J. Lachaud
η(-), Kn	Tortuosity, Knudsen number	Diffusiometer	AD	E. Stokes
		Tomography + DNS	AM	E. Dickey/J. Lachaud
Conservation of Energy				
h_{mat}, h_{fiber} (J/kg)	Enthalpy of the solid	DTA/DSC	SoA/AD	J. Feldman
k (W m^{-1} K^{-1})	Effective conductivity	Flash	SoA	J. Feldman

SoA: state-of-the-art / AD: additional data / AM: alternative method.

Experimental Characterization Methods for Three-Dimensional Microstructure Analysis

Elizabeth C. Dickey, North Carolina State University, USA

Incorporating material microstructure, i.e. porosity and phase distribution, into ablation modeling requires the input of quantitative three-dimensional experimental microstructure across multiple length scales. These experimental data are critical to define the initial-state of the material and to validate model predictions of microstructural evolution. This talk will review current experimental capabilities for three-dimensional microstructural analysis based on optical, x-ray and electron scattering. The applicability of the various techniques for measuring surface roughness and three-dimensional microstructure of ablative materials will be discussed. Comparisons will be made between resolution, field-of-view and the non-destructive nature of the techniques.

Internal Reactions in Porous Carbon Chars – Flow-Tube Reactor Approach

Eliza Jochen Marschall, SRI International, USA

A flow-tube reactor approach to study gas-surface reactions on carbon will be described. Experiments on carbon oxidation and nitridation will be presented, and proposed experiments to document pyrolysis gas chemistry in hot carbon chars will be discussed. Flow tube reactor experiments use simple axisymmetric geometries amenable to direct modeling with minimal approximation. The presentation will focus on the control and verification of test conditions, and on the available measurement techniques for quantifying reactant and product concentrations. In particular, we will discuss the generation and quantification of dissociated oxygen and nitrogen using discharge sources and titration techniques, and their detection by laser induced fluorescence, as well as the use of mass spectrometry to study the chemical evolution of pyrolysis gas mixtures.
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Characterizing Ablator Properties – Review of Some Techniques and Challenges in Obtaining Meaningful Data

Jay Feldman & Mairead Stackpoole, ERC Inc, USA

Adequately characterizing the ablative Thermal Protection System (TPS) of an entry vehicle is critical to TPS model development and vehicle design. Understanding the nature of the ablative TPS, it's inherent construction and variability, are crucial prerequisites to obtain accurate and meaningful property data. Some examples of ablator systems and the inherent challenges they pose to characterization will be reviewed. The question of how to obtain properties for char will also be addressed. Techniques for measuring thermal conductivity and enthalpy will be presented, and the uncertainties, advantages and challenges in applying these techniques to various ablator systems will be discussed.

Mass Spectrometry of Pyrolysis Products during Thermal Decomposition of Ablator Materials

Jason D. White, Jochen Marschall, SRI International, USA

Mass spectrometry is a powerful technique for the characterization of pyrolysis gas composition during the thermal decomposition of ablative materials. Coupling a mass spectrometer to a thermogravimetric analyzer allows for relatively straightforward *qualitative* identification of chemical species and their correlation with mass loss during heating. However the *quantification* of species in a pyrolysis gas mixture is a much more difficult task.

In this presentation, we will review different aspects of mass spectrometry including gas sampling approaches, species ionization methods, and ion measurement techniques. We emphasize the advantages of time-of-flight (TOFMS) over quadrupole (QMS) ion separation because of its fast response time and the ability to capture an entire mass spectrum after every ionization event. The most ubiquitous ionization method utilizes 70eV electron impact (EI) ionization to generate ions, which can be used to identify molecular compounds. One complication of this technique is that molecules generally undergo significant fragmentation, which makes identification and quantification of parent species from complex and overlapping fragmentation patterns extremely difficult for complex gas mixtures. The use of single photon ionization (SPI) minimizes fragmentation and generates much 'cleaner' spectra, albeit only for species with ionization energies less than the incident photon energy.

We will describe our attempts to combine both EI-QMS and SPI-TOFMS to measure and quantify the decomposition products of characteristic ablator materials, including the development of a quantification method based on a benzene standard and a "ladder" quantification procedure to evaluate the gas-phase mole fractions of decomposition products. The results of this preliminary approach will be presented, the challenges of quantification will be discussed, and suggestions will be made for future experimental designs that utilize improved analytical instrumentation.

Using FT-IR Spectroscopy to Elucidate the Structures of Ablative Polymers

Wendy Fan, ERC Inc, USA

The composition and structure of an ablative polymer has a multifaceted influence on its thermal, mechanical and ablative properties. Understanding the molecular level information is critical to the optimization of material performance because it helps to establish correlations with the macroscopic properties of the material, the so-called structure-property relationship. Moreover, elucidation of the molecular structure is also essential to predict the thermal decomposition pathways as well as to identify decomposition species that are fundamentally important to modeling work. In this presentation, I will illustrate the use of infrared transmission spectroscopy (FT-IR) as a convenient tool to elucidate the structures of several major classes of ablative polymers.

Measurement of Mass Transport Properties of Carbon Phenolic Ablator Materials and Their Relationship to Material Behavior in Use Environments

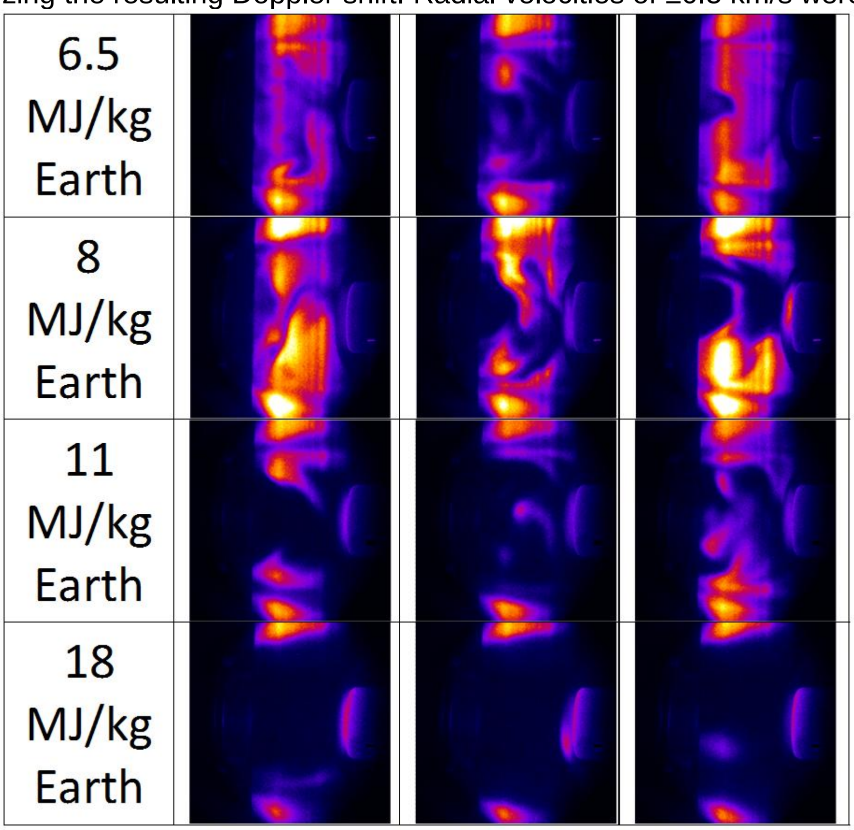
Eric Stokes, Southern Research Institute, USA

Several types of anomalous behavior have been observed with phenolic based ablatives in post-fired nozzles, exit cones, and reentry vehicles. Many of these events have been shown to be related to the development of internal gas pressure within the material during use. The development of internal gas pressure is a function of the amount of gas produced within the material and the rate at which that gas is allowed to escape. The former is controlled by the material's temperature, the kinetics of chemical conversion of the phenolic resin, and possibly the internal gas pressure itself. The latter property of a material is referred to as the material's permeability and as such is independent of specimen geometry, pressure differential, and properties of the gas being transported. The permeability of carbonized fiber based phenolic composites is a function of material direction, temperature, temperature history, constituent composition, processing, and the stress-strain state of the material. Other variables like the environmental history of the material prior to use may also affect the subsequent development of porosity in the material during use. This paper examine why we think these variables are important in modeling the behavior of phenolic based materials in their use environment.

Nitric Oxide PLIF Measurements in the Hypersonic Materials Environmental Test System (HYMETS)

Paul M. Danehy, NASA Langley Research Center, USA

A nonintrusive laser-based measurement system has been applied for the first time in the HYMETS (Hypersonic Materials Environmental Test System) 400 kW arc-heated wind tunnel at NASA Langley Research Center. Planar laser-induced fluorescence of naturally occurring nitric oxide (NO) has been used to obtain instantaneous flow visualization images, and to make both radial and axial velocity measurements. Results are presented at selected facility run conditions, including some in simulated Earth atmosphere (75% nitrogen, 20% oxygen, 5% argon) and others in simulated Martian atmosphere (71% carbon dioxide, 24% nitrogen, 5% argon), for bulk enthalpies ranging from 6.5 MJ/kg to 18.4 MJ/kg. Flow visualization images reveal the presence of large scale unsteady flow structures, and indicate nitric oxide fluorescence signal over more than 70% of the core flow for bulk enthalpies below about 11 MJ/kg, but over less than 10% of the core flow for bulk enthalpies above about 16 MJ/kg. Axial velocimetry was performed using molecular tagging velocimetry (MTV). Axial velocities of about 3 km/s were measured along the centerline. Radial velocimetry was performed by scanning the wavelength of the narrowband laser and analyzing the resulting Doppler shift. Radial velocities of ±0.5 km/s were measured.



Typical PLIF images of naturally occurring nitric oxide present in the freestream of the HYMETS facility. Flow is from left to right. Three single shot images are shown for each of four different flow enthalpies.

The images indicate that the flow is nonuniform in the freestream, and that the nitric oxide concentration decreases at enthalpy increases.

GAS-SURFACE INTERACTION AND CATALYSIS
CHAIRS: MATTHEW MACLEAN AND JOCHEN MARSCHALL

Return of Hayabusa Sample Return Capsule and Japanese Ablator Technologies

Tetsuya Yamada, Japan Aerospace Exploration Agency, Japan

I would like to summarize the return of the Hayabusa Sample Return Capsule especially from the aerothermal point of view. The topic will be followed by a brief introduction on ablator analysis by Japanese TPS researchers for future missions.

Investigation of the Gas-surface Interaction of Innovative Carbon Composite Ablators in the VKI Plasmatron

O. Chazot, B. Helber, C. Asma, Y. Babou, T. Magin, Von Karman Institute, Belgium

For a new class of low density carbon/resin composite ablators, which has been introduced and successfully applied to flight by the Stardust mission, the process of ablation is not only restricted to the surface but can also occur in-depth of the material if oxygen is able to diffuse into the porous material. The occurrence of such new porous carbon/resin composites requires an important effort in theoretical and experimental investigation for an adequate understanding of the ablation process to enable development and validation of material response models. At the von Karman Institute for Fluid Dynamics (VKI) research activities were developed to establish a methodology for experimental characterization of innovative low-density ablators using the inductively coupled 1.2MW Plasmatron facility. A comprehensive setup of measurement techniques was applied to the facility in order to determine and characterize the in-situ material response of ablative samples in different test conditions. Optical emission spectroscopy was utilized to address the thermo-chemistry of the plasma free-stream and its interaction with the ablating sample. In addition microscopic analysis tools for sample examination, at the carbon fibre length scale (~10μm), are used to investigate the material physics. The degradation behaviour of the material is then being analyzed by scanning electron microscopy to be able to evaluate the depth of degradation and the thinning of the carbon-fibres. In particular, to provide information about the diffusion/reaction competition of oxygen, which controls the oxidation of carbonized resin and exposed fibres in-depth. Material surface properties, as emissivity, are also determined in-situ using an IR-radiometer combined with two-colour pyrometer measurements. Preliminary results showed that nitridation, leading to CN (CN violet & CN red), is highly apparent in pure nitrogen plasma flows but significantly drops when oxygen is involved, speaking for dominant oxidation reactions (CO, CO2, NO). Additionally, different chemical mechanisms were found to occur rather in nitrogen than in air plasma. In such a way, diatomic carbon (C2 Swan) transitions were highly radiating after injection of the sample into N2 plasma but truncated after a few seconds. This was not observed with air as test gas. As expected, oxygen is the driving force to provoke reactions as the system undergoes the ablation process, but its uncertain state of diffusion into the porous material and on the contrary, reactions undergone in the absence of oxygen, necessitate the usage of appropriate micro- and spectroscopic tools.

Gas-Surface Interaction Measurements in the 30kW ICP Torch Facility

Douglas Fletcher, University of Vermont, USA

A series have tests have been conducted in the 30 kW ICP Torch Facility at the University of Vermont with the goal of obtaining a measurement of the graphite nitridation rate. This reaction is important for carbon-based heat shields in many planetary entry applications. Graphite also represents a simplified ablator, as the material is relatively homogeneous and the surface will recess without pyrolyzing. The measurements were made using laser-induced fluorescence (LIF) of the nitrogen atoms in the near-wall region along the stagnation streamline. These spatially resolved measurements provided values of the local translational temperature and relative atom number density. Additional measurements are ongoing to convert the relative measurements to absolute values. The gradient in atom concentration provides a qualitative indication of the reaction efficiency at the surface, while the absolute values allow a quantitative estimation of the reaction efficiency. Results from these tests are presented and discussed and additional activities supporting an investigation of pyrolysis are summarized.

High Enthalpy Ablation Testing at DLR Cologne

B. Esser, A. Gülhan, U. Koch, German Aerospace Center (DLR), Germany

Testing thermal protection capabilities of ablative materials is one of the main working areas of DLR's arc heated facilities LBK in Cologne. Work on this particular topic has been intensified about five years ago with the following major focus points:

- Significant improvement of the facilities testing capabilities with respect to cold wall heat flux rates and stagnation pressure.
- Ablation testing in Martian atmosphere.
- Influence of dust particle erosion on ablation.

With a new nozzle the testing capabilities at LBK could significantly be improved. Cold wall heat flux rates up to 12 MW/m2 can be reached at stagnation pressures up to 1500 hPa. These conditions have already been used intensively for the characterization of new ablative materials within ESA projects as well as in direct commission of European space industry. The corresponding flow field around a flat-faced cylinder model was characterized by single pulse broadband Coherent Anti-Stokes Raman Scattering (CARS). Vibrational and rotational temperatures were measured simultaneously with this technique identifying thermodynamic non-equilibrium for both, free stream and shock layer.

When planning interplanetary missions to Mars with a direct entry into the atmosphere the possibility of being exposed to a dust storm must be taken into consideration. Therefore, thermal protection systems have to be designed for sustaining higher loads caused by dust particle erosion. In the frame of three studies under the lead of ESA and CNES several test campaigns were performed to investigate the influence of particle erosion on the Norcoat Liege ablator, which will be used as heat shield for the EXOMARS missions. Tests were carried out at several flow conditions imposing different heat loads on the samples. Particle velocities up to 2 km/s could be achieved. Particle deceleration in the shock layer was measured using the Laser-2-Focus (L2F) technique. Based on the erosion results a new particle erosion correlation could be developed for Norcoat Liege.

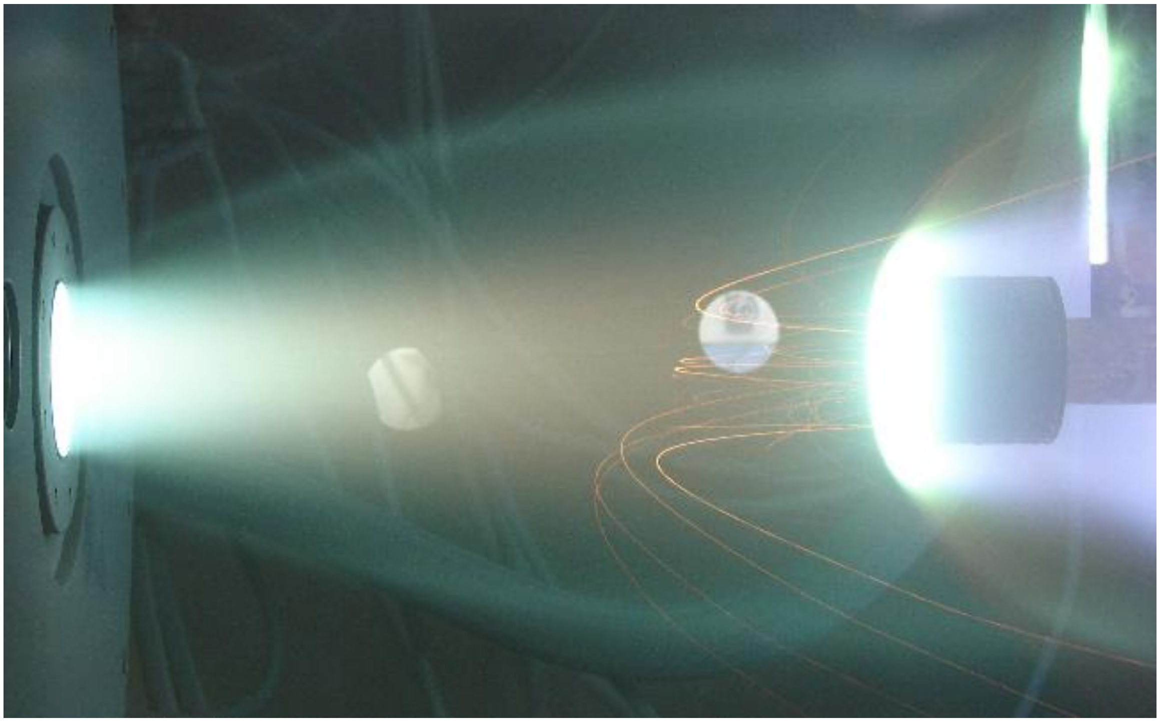


Figure: Ablator sample in dust loaded CO2/N2 flow

GSI Modeling Overview: Requirements for Macroscopic Gas/Surface Interaction Coupling to CFD Codes

Matthew MacLean, CUBRC, USA and Jochen Marschall, SRI International, USA

An overview is presented of a generalized finite-rate surface chemistry model that has been developed for gas/surface interaction coupling to the Data-Parallel Line-Relaxation (DPLR) code. Species from the gaseous environment are allowed to interact with species adsorbed onto one or more phase of a surface and with one or more phases of a bulk thermal protection system through an arbitrary number of finite-rate reactions. The reactions may include types such as adsorption, desorption, Eley-Rideal recombination, Langmuir-Hinschelwood recombination, partial or total dissociative adsorption, oxidation, reduction, sublimation, or condensation where forward and reverse rates are constrained by thermodynamics. A simple pyrolysis model is incorporated into the gas species mass balance and energy balance boundary conditions where the pyrolysis production may be specified explicitly from an uncoupled material response analysis or assumed steady-state proportionality to the bulk phase ejection rate. The production rates of all gaseous species are implicitly coupled into the viscous wall boundary condition of the DPLR code to maximize the convergence rate of the solver. Examples are shown for a catalysis system and a TPS system to demonstrate the model. The focus of the work presented is primarily to demonstrate the necessary model, reaction, surface, and material data required.

II. Gas/Surface Interactions (GSI) and Catalysis

Model Parameter	Parameter List / Options / Needs
Allowed GSI phases	One gas phase, multiple surface phases (multiple sets of active sites in each, multiple bulk (TPS) phases)
Types of allowed reactions	(1) Adsorption/desorption, (2) Eley-Rideal/ partial dissociative adsorption, (3) Langmuir-Hinshelwood/dissociative adsorption, (4) Oxidation/reduction, (5) Sublimation/condensation
Surface reaction data	Forward rate coefficient for each surface reaction
Thermodynamic data	Gibbs energy curve fits for each gas and bulk species; specified equilibrium constant or desorption rate for each adsorbed species
Surface phase data	Surface fraction for each surface phase; active site density (in mol/m^2) for each active site set in each surface phase
Bulk phase data	Volume fraction, mass density, and porosity for each bulk phase; species composition of each bulk phase
Pyrolysis data	Specified pyrolysis gas mass flow rates and species composition
Number of surface phases &area fractions	Reflect the composition and microstructure of TPS :manufacturing info and microscopy
Number of active site sets/phase	More than one type of surface site required to model important reactions?
Active site density of each set	Should reflect atomic-scale structure of surface: (x-ray diffraction, Leed/Rheed, Raman, Auger, STM/AFM, etc.) Should reflect expected species-surface interactions: (UHV surface science experiments and ab initio chemistry calculations)
Number of bulk phases &volume fractions	Reflect the composition and microstructure of TPS : (manufacturing info, microscopy)
Species and composition in each phase	Chemical composition of TPS constituents: (manufacturing info, chemical analysis)
Mass density and porosity	Physical measurements: weight, volume, density, porosimetry

Reactions

Adsorption/Desorption
Sticking coefficients
Energy Barriers
Adsorption and desorption

Arrhenius Reactions
Pre-exponentials
Energy barriers

Kinetic Reactions
Sticking Coefficients
Sublimation Coefficients
Reaction Efficiencies

Energy barriers
Surface Diffusion
Recombination and desorption
Condensation and sublimation

Sources

Chemical literature:
- Bond strengths
- Dissociation energies
- Reaction mechanisms

Experiments:
- Adsorption Isotherms (BET)
- Temperature-Programmed Desorption (TPD)
- Molecular beam experiments
- Flow tube/diffusion reactors

Simulations:
- Density-functional theory
- Kinetic Monte-Carlo
- Others

Surface Catalysis Measurements Using a Diffusion-Tube Side-Arm Reactor

Jochen Marschall, SRI International, USA

The theory and application of the diffusion tube side-arm reactor technique for characterizing surface catalytic recombination reactions will be described. In this technique, reactants diffuse into a dead-end tube and are progressively removed from the gas phase by surface reactions on the walls, establishing unique steady-state concentration profiles along the length of the tube. Reactant loss probabilities are determined by matching experimentally measured species profiles to calculated solutions of a reaction-diffusion model. The advantages of laser-based methods for species concentration measurements are summarized and different approaches to reactor modeling and the extraction of reaction efficiencies from measured data are presented. The advantages and limitations of the diffusion-tube side-arm technique, the associated uncertainties in derived loss probabilities, and the prospects for further laboratory development, are presented.

Oxidation Behavior of Ultra-High Temperature Ceramics Using Different High-Temperature Test Facilities

Joch Erica L. Corral, Melia Miller, Luke S. Walker, David Pham, and William Pinc, The University of Arizona, USA

The development of advanced thermal protection system (TPS) materials for use in next generation aerospace vehicles is needed. Ultra-high temperature ceramics (UHTCs) are considered viable candidates for hypersonic vehicle TPS materials due to their high melting temperature and good thermal conductivity. However, the need for new TPS materials has also prompted the need for the development of relevant test methods that simulate flight environments. Therefore, the focus of this talk will be to investigate the effect of high temperature test facility environments on the oxidation behavior of UHTCs. Three testing methods will be used to assess UHTCs at high temperatures (up to 2000 °C) and heat flux up to 200 Wcm^{-2}. The first is an oxyacetylene torch set up according to ASTM E285-80 with oxidizing flame control and maximum achievable temperatures in excess of 2000 °C. The other two are high temperature static oxidation furnaces such as a thermal gravimetric analyzer and a box furnace capable of operating up to 1650 °C. The former is capable of *in situ* detection of weight loss and weight gain due to oxidation of the material under controlled high temperature gas mixtures thus allowing us to measure oxidation rates. In this study, ZrB_2-SiC composites were processed using spark plasma sintering and were evaluated for oxidation behavior using our high temperature test facilities. The test facilities will be discussed in detail and correlated with preliminary materials evaluation results. We will also discuss collaborative testing efforts (plasma, solar furnace, and hyperthermal oxygen atoms) and on going development work at UA (dissociated air mixtures) in order to further develop an understanding for the effect of test environment on oxidation behavior of UHTCs.

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Characterizing TPS Microstructure – Review of Some Techniques to Capture and Quantify Scale of Microstructure

Mathew Gasch, NASA Ames Research Center, USA

Adequately characterizing the Thermal Protection System (TPS) of an entry vehicle is one of the key components of vehicle design. Lightweight charring ablative materials such as PICA and SIRCA consist of a porous matrix filled with a polymeric ablative component. These materials have highly porous microstructures (>80%). Characterizing the scale of the porosity, the surface area of the various phases and the morphology of the polymeric components is insightful and necessary to support model development. This presentation will highlight techniques useful in characterizing these ablators with emphasis on Scanning Electron Microscopy (SEM) and Accelerated Surface Area and Porosimetry System (ASAP).
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In-Situ Techniques to Understand Changes in Surface Chemistry During Ablation

S.M. Aouadi, D.S. Stone, C. Muratore, A.A. Voevodin, Southern Illinois University, USA

Ablation is an effective and reliable method largely used in aerospace structures to protect the payload from damaging effects of external high temperatures. Substantial research is required to develop basic knowledge that is required to characterize the response of a high temperature thermal protection system to extreme hypersonic environment. This presentation will provide an overview of experimental techniques that are currently being used to understand the degradation behavior of composite materials used for thermal protection. Advantages and disadvantages of each method will be discussed. In addition, novel *in situ* quantitative methods of material degradation during high temperature ablation events will be identified. Specific techniques developed by the authors for hypersonic applications will be discussed. For example, *in situ* Raman spectroscopy during high temperature wear testing of chameleon coatings was employed by the lead author to correlate surface chemistry to measured changes in friction coefficients simultaneously. Chameleon coatings are adaptive coatings that reduce friction coefficient from 25 to 1000 °C for moving assemblies for next-generation hypersonic aircraft and missiles.

Atomistic to Macroscopic Modeling and Validation for Gas-Surface Interactions

T. E. Schwartzentruber, University of Minnesota, USA

The high-temperature shock layer generated by a hypersonic vehicle results in the dissociation of free-stream diatomic and polyatomic molecules. These reactive atomic species may diffuse through the boundary layer and recombine back into molecules on the vehicle surface (catalysis) or actually react with and remove material from the surface (ablation). Efforts are underway to develop a finite-rate gas-surface-interaction model, incorporated as a CFD boundary condition, in order to reduce the uncertainty in predicted heat flux associated with these phenomena.

An important aspect of the finite-rate model is that it consists of a set of one-step (elementary) gas-surface chemical reaction mechanisms with parameterized rates. Unlike prior models parameterized by overall recombination coefficients or overall oxidation rates, for example, the parameters required by the new model have a quantitative link to *individual* surface chemistry mechanisms. Although such parameters may be partially informed by existing experimental data and chemistry theory, the uncertainty is quite large. A suggested approach is to first apply uncertainty analysis to a given finite-rate model to determine the dominant mechanisms (and associated parameters) that contribute to the predicted heat flux. Followed by targeted computational chemistry simulations and experimental measurements to reduce the uncertainty in specific parameters of interest.

Techniques for simulating molecular beam experiments to determine parameters such as sticking coefficients, reaction efficiencies, scattering angles, and energy accommodation coefficients, will be presented. Techniques for predicting surface coverage at various (r_i, p, T) conditions will be presented and compared to low-energy electron diffraction (LEED) and temperature-programmed desorption (TPD) experiments, as well as scanning tunneling microscopy (STM) images. Finally, techniques for simulating activation energies for E-R/L-H recombination and oxidation reactions will be presented.

Current results are for well-characterized model systems (Pt(111), silica-quartz). Extension to simple carbon surface ablators under flight-relevant conditions will be discussed along with associated challenges.

ROUGHNESS MODELING WITH GAS BLOWING EFFECTS
CHAIRS: ADAM AMAR AND CHARLES POWARS

Overview of Roughness and Blowing Effects in Flows Over Ablating Surfaces

Adam Amar, NASA Johnson Space Center, USA and Charles Powars, St. Croix Research, USA

The scope of this session includes ablation effects on surface roughness and surface roughness effects on ablation. Ablation involves blowing, and so we address blowing including combined roughness and blowing effects. The two distinct types of ablating material surface roughness are defined with examples: 1) roughness related to the material inhomogeneity, and 2) roughness induced by turbulent flow that appears to be unrelated to material inhomogeneties.

Existing approaches for modeling ablative material surface roughness and blowing effects are overviewed. These range from empirical “augmentation factor” correlations to high-fidelity simulations of flow-surface interactions using modern CFD techniques. For models requiring input of roughness morphology information (e.g., effective sand grain roughness height), potential experimental and analytical sources of this information, and associated challenges, will be discussed. With regard to all modeling approaches for predicting ablative material surface roughness and its effects, experimental strategies for generating data needed for model development and validation will be emphasized.

Open questions for development of physics based roughness models	Target experimental objectives
• What kind of surface roughness (i.e., roughness height and character) develops on ablating materials, and how does this depend on material and environment parameters? • What determines when flow-induced ablation patterns (e.g., striations, crosshatching, scallops) do and do not develop? • Can the effects of flow-induced ablation patterns on heat and mass transfer rates be accounted for using models developed from artificial (e.g., machined) roughness data? • How do roughness and blowing effects on heat and mass transfer combine? Can we model these effects independently? Must experiments simultaneously simulate roughness and blowing? • How does surface roughness affect laminar flow heat and mass transfer (i.e., other than the effect on boundary layer transition), and how should this effect be modeled? • For blunt bodies over which the flow is assumed to be turbulent, how should we interpret and model surface roughness effects on stagnation point heat and mass transfer? • What is the most appropriate way to account for surface roughness and blowing effects in the CFD and material ablation analysis tools used for heatshield design?	• Cleverly designed experiments that address the "open questions" are needed • Example experimental approaches and challenges: 1. Rough-wall heat transfer models tested in hypersonic wind or shock tunnel – Facilities with adequate turbulent flow Re, M, size, etc.? – Relating machined model roughness to ablating material roughness? – Rough wall heat transfer instrumentation difficulty? – Fabrication of instrumented models with roughness & blowing? 2. Ablation materials of interest tested in hyperthermal facility – Candidate facilities: arc heaters, ballistics ranges, rockets, other? – Ability to provide appropriate turbulent flow ablation environment and test duration (particularly for blunt bodies)? – How to isolate surface roughness effects from other heat transfer and ablation uncertainties? – How to characterize surface morphology; in situ, post-test? 3. Low-temperature ablator models tested in hypersonic wind tunnel – Facilities with adequate Re, M, size, run time, etc.? – Can LTAs simulate ablative TPS roughness? – Can surface roughness and blowing effects be accurately inferred from ablation data?

Fundamental Studies of Surface Roughness and Ablating Flows

Ada R. Bowersox and S. North, Texas A&M University, USA

National interest in hypersonic flight provides the motivation to develop closure models for high-speed turbulent boundary layer flows with mechanical, thermal and chemical non-equilibrium effects. Our approach toward developing the required models is based on algebraic truncations to the second-order turbulent transport equations, which include non-equilibrium effects. One of the major challenges associated with developing these models is a lack of experimental information to verify assumptions and validate performance. In this presentation, we will describe (1) the results from a series of experimental studies focused on providing improved understanding of the effects of roughness on the structure of the turbulent boundary layer and (2) plans for upcoming experiments characterizing heat transfer and surface ablation. For the roughness studies, high-fidelity experimental characterizations of the turbulence response to both global and local non-equilibrium were performed at Mach 3.0 and 5.0 using particle image velocimetry. These studies are providing new insights into the fundamental differences between supersonic and subsonic mechanical non-equilibrium flows, as well as guidance for assessing turbulence model applicability. A large part of our recent efforts have focused on developing new laser based diagnostics and hypersonic facilities to extend our experimental methods to include flows with ablation. Specifically, we have developed a new diagnostic to enable temperature, velocimetry and concentration measurements. In this presentation, we will discuss our approach and show representative results.

Heat Transfer Measurements to Examine Surface Roughness and Blowing Effects in Hypersonic Flows

Michael S. Holden, Erik P. Mundy, and Matthew MacLean, CUBRC, Inc., USA

Experimental studies have been conducted in the LENS supersonic and hypersonic tunnels to examine surface roughness and blowing effects on the heating and skin friction to blunt nosetip and slender blunted cones in regions of laminar, transitional and turbulent flows. Heat transfer measurements have been made on rough surfaces, and smooth and rough porous surfaces, with specially designed and constructed thin-film and calorimeter instrumentation. The rough surfaces employed in these studies were constructed with both sand grain roughness and patterned roughness with well-defined surface geometries constructed with hemispherical and conical roughness elements. The spacing of the hemispherical and conical roughness elements were varied to obtain measurements with which to generate correlations of the roughness-induced heating enhancement in terms of parameters which characterize the surface geometry of the rough surfaces. The well-defined geometric character of the patterned roughness also provides well-defined boundary conditions for future computations that compute the flow over the roughness elements. Unique thin-film heat transfer instrumentation and rough porous surfaces have been constructed and employed to examine the separate and combined effects of surface blowing on the heat transfer to these surfaces in laminar, transitional and turbulent flows. The measurements made in these studies have been analyzed to correlate the roughness-enhanced heating with the height, shape and spacing of the surface roughness and the freestream conditions. The results of this analysis suggest that roughness augmented heating cannot be correlated simply in term of roughness Reynolds number. Our correlations of the effective roughness height with shape and spacing parameters differ significantly from measurements in subsonic flows. The heat transfer and skin friction measurements made with surface blowing on a blunted cone for a series of different gaseous injectants have been correlated with a blowing parameter which incorporates the molecular weight and specific heat of the injectant. These correlations indicate that surface roughness effects persist to relative high blowing rates. During these studies, we employed high-frequency thin-film instrumentation to measure the heating rate in the stagnation regions of the flow and concluded that in high Reynolds number flows, heating enhancement can result from disturbances to the boundary layer in the stagnation region originating from tiny particulates in the freestream.

Roughness Induced by Chemical Ablation in Carbon Based Ablators: Onset and Macro-Scale Handling

Yvan Aspa, Jean Lachaud, Gérard Vignoles, Michel Quintard, Astrium ST, France

Roughness of heat-shield materials has been studied in the frame of aerodynamics and the laminar-turbulent transition through a wide range of experimental and numerical works. On the contrary, the dynamic link between chemical ablation and roughness has been poorly tackled. In the present work, the role of chemical reaction in the onset, development and stabilization of composite roughness is exposed. A second part is dedicated to the handling, at macro-scale, of an heterogeneous rough reactive surface.

By design composites are chemically non-uniform. At surface, this property leads to a different behavior of the material components with respect to the oxidants brought by the surrounding flow. A minimal micro-scale model coupling diffusion and reaction is used to illustrate roughness evolution from onset to stabilization. The use of 3D numerical simulation feeds numerical experiments that are successfully compared to SEM observations.

At TPS scale, the chemical reactions leading to ablative mass loss are seen as being purely surfacic. Indeed as classical roughness pattern is two or three magnitude scale smaller than the vehicle, a direct handling is not a suitable approach. In order to take into account the effect of roughness, an upscaling of the phenomenon occurring at micro-scale is proposed. This procedure uses a domain decomposition technique. The theoretical transformation of equations allows building, through closure relations, an explicit link between micro-scale reaction and macro-scale mass loss. In this study, the theoretically obtained relations are validated by comparing a direct numerical simulation and the homogenized problem.

A Combined Numerical and Experimental Investigation of the Coupling Mechanisms Between an Ablative Wall and Turbulence

Christopher White, University of New Hampshire, USA and Yves Dubief, University of Vermont, USA

This talk will describe a collaborative effort between numerical simulations and experiments to investigate the fundamental coupling mechanisms between an ablative wall and turbulence. The scientific approach employed is to systematically validate numerical and experimental methods and advance our understanding of the phenomenon as a progression from simple flows to turbulent flows. The flow configuration studied is a spatially developing heated boundary layer flow over a wall made of transparent paraffin wax. Several variations of the inlet conditions, both for flow and temperature, will be described that will allow for the temporal and spatial study of the ablation processes driven by coherent structures, such as vortices, and the response of turbulence to wall recession and emergence of roughness (ablation patterns). The choice of paraffin wax as the ablated material is based on its low melt point temperature and its ability to ablate in two phase steps (solid to liquid, and liquid to vapor, if the flow temperature is high enough), which is necessary for the development of our numerical algorithm. The focus of the talk is to provide a description of the experimental facility, experimental methods, numerical models, planned experiments, and preliminary results.

Prospects for DNS and LES of Ablating Surfaces

Graham V. Candler, University of Minnesota, USA

The interaction of a turbulent boundary layer with an ablative surface is known to produce cross-hatching and scalloping of the surface under certain conditions (e.g. Grabow and White 1975). These patterns are known to increase the convective heating and the rate of ablation. Recent developments in low-dissipation high-order numerical methods, computational grids, and large-scale computation promise to make it possible to directly simulate flows at relevant high-enthalpy conditions. In this talk we discuss the prospects and requirements for using these high-fidelity simulations to fully understand surface pattern formation under turbulent flow conditions. Examples of recent simulations will be used to illustrate the potential of this approach.
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Spatially and Temporally Resolved Data of High Enthalpy Turbulent Boundary Layers

Pino Martin, University of Maryland, USA

Enabling high fidelity simulations of entry and re-entry turbulent flow environments requires the generalization of scaling laws and new fundamental understanding describing the interaction of turbulence with shock waves, finite-rate reactions, surface catalysis and ablation, and radiation. The use of direct numerical simulation data to extend turbulence scaling and advance turbulence models for high enthalpy conditions will be described, including on-going work to account for surface catalysis, roughness, and blowing and transpiration that is found in ablating environments.

Simulation of Roughness Effects on Hypersonic Blunt Body Entry Heating

Yehia Rizk, NASA Ames Research Center, USA

The objective of the current work is to improve Computational Fluid Dynamics (CFD) prediction of turbulent heating in the presence of distributed surface roughness. Typically, distributed surface roughness is encountered in earth or planetary entry of spacecraft with ablative heat shields. The current approach is based on the use of a combination of CFD analysis and experimental observations to improve the turbulence modeling needed to predict the effects of roughness on turbulent surface heating. Several experiments are used to guide as well as validate proposed modification to the commonly used Baldwin-Lomax turbulence model to improve its prediction of heat transfer in the presence of surface roughness. Specifically, the current work describes two different modifications to the inner layer of the Baldwin-Lomax model. The modifications are implemented in the DPLR code but could be easily utilized in any CFD code that uses the Baldwin-Lomax model. The proposed modifications are consistent with similar modifications developed earlier to treat surface mass injection. This has the potential to eventually develop a model capable of treating combined roughness and surface blowing. Heat transfer data obtained from both the original and modified roughness models are compared with several heat transfer data obtained from available experiments with surface roughness corresponding to values encountered during flight conditions. The results clearly show that the proposed modification produce a much better prediction of the heating augmentation due to surface roughness.

ABLATION MODEL CODE INTERCALIBRATION EXERCISE
CHAIRS: BERNIE LAUB AND ALEXANDRE MARTIN

NASA Engineering Safety Center Thermal Performance Database

R. French, J. Grimes, M. Grover, D. Hash, T. Huang, J. Tran, M. Wright, NASA, USA

Thermal performance testing and analysis costs are high and represent a significant technology investment. Currently, the test data, even for a single test, typically resides in multiple locations leading to excessive effort by members of the thermal performance community when collecting and validating data. Recognized as a valuable investment in data archiving and the thermal performance test process, the NASA Engineering and Safety Center (NESC) has chartered the development of the Thermal Performance Database to create a centralized, query capable repository of thermal performance test and analysis data. Including available historical data and designed to be an integral element in future thermal performance testing, the database is currently under the initial stages of development with a planned first deployment in 2011.

Presentation of the 2011 Ablation Test Case

Jean Lachaud (UC Santa Cruz), Alexandre Martin (University of Kentucky), Ioana Cozmuta (ERC), and Bernie Laub (NASA Ames)

Objectives

Three types of material-response codes have been identified in the community:
Type 1: CMA-type codes (heat transfer, pyrolysis decomposition, simplified transport of the pyrolysis gases, equilibrium chemistry);
Type 2: CMA model augmented with an averaged momentum equation for the transport of the pyrolysis gases;
Type 3: Higher fidelity codes (possibly including finite-rate chemistry, multi-component diffusion, etc).
A test case with two objectives has been defined:
1. Inter-calibration of codes of the same type (focus: numerical methods and data interpretation);
2. Comparison of codes of different types (focus: modeling approach).

2011 Test case

For this first inter-comparison exercise, a simple one-dimensional test case without surface recession has been defined. The goal is to compare the in-depth physics and chemistry models implemented in the codes. A fixed temperature of 1644K and a fixed pressure of 1 Atm are imposed on one end of a five-centimeter sample of charring material. On the other end, the sample is assumed adiabatic and impermeable. The duration of the test is one minute. The initial conditions are as follows: temperature of 298K, atmospheric pressure. The initial gas composition in the material is left open. The charring material of the 2011 test case is a theoretical low-density fibrous ablator, called TACOT (Theoretical Ablative Composite for Open Testing). The properties of this material have been defined using literature data to enable open diffusion. Input data needed for the three types of codes are furnished: composition and microstructure, thermal properties, transport properties, pyrolysis model, finite-rate chemistry of the pyrolysis gases, thermo-chemical properties. The participants may use all or parts of the furnished properties. A baseline solution from a type 1 code (FIAT) is provided. Participants are invited to plot their results against the baseline for visual comparison and are invited to discuss them during the workshop [5 minute presentations and posters]. Participants are also invited to provide their output file for statistical analysis by the NASA Thermal Performance Database (TPDB) team [15 minute presentation].

Outlook

More elaborated test cases will be defined for next year (surface recession, multi-dimensional) and will be discussed at the end of the session [15 minute discussion].

Presentation of the 2011 FIAT Baseline Results

Bernie Laub (NASA Ames) and Ioana Cozmuta (ERC Inc)

The workshop organizers defined a relatively simple case for this initial code intercalibration exercise. The analysis objective is to calculate the thermal and in-depth thermochemical response of a 50 mm thick fictitious low-density phenolic-reinforced carbon composite called TACOT (Theoretical Ablative Composite for Open Testing). The surface boundary condition is for a 60 s exposure to a constant 1644 K surface temperature. The back wall boundary condition is adiabatic. Virgin and char thermal properties for TACOT are defined as are decomposition kinetics. Pyrolysis gas molar composition is defined and the enthalpy of the pyrolysis gas assuming thermochemical equilibrium at a pressure of 1 atm is provided, although participants are free to use different assumptions or more sophisticated modeling. Surface themochemistry and surface recession are not considered for this case.

The CMA code has been the industry standard for the past 40 years. The FIAT code, developed at NASA Ames, is an upgraded version of CMA. A FIAT analysis was conducted using the properties provided to define baseline results for code comparisons. Additional FIAT cases were run to demonstrate the influence of specific characteristics of this problem. For example, the assumption of an equilibrium pyrolysis gas enthalpy results in an unrealistic exothermic pyrolysis process whereas use of literature values for the heat of pyrolysis can be implemented. These baseline results will be available for comparison with analysis results from other codes.

ABLATION CODES INTERCALIBRATION RESULTS

MOPAR: Results of the Inter-code Calibration of Charring Material Response

Alexandre Martin, University of Kentucky, USA and Jonathan Wiebenga & Iain D. Boyd, The University of Michigan, USA

As the part of an ongoing study on heat flux and ablation on hypersonic vehicles, a one dimensional material response implicit solver with solid ablation and pyrolysis has been developed at the University of Michigan. This code, named MOPAR, uses the Control Volume Finite-Element Method (CVFEM) to model surface ablation with wall recession, as well as inner decomposition and pyrolysis gas behavior. The code solves the solid and gas phase mass conservation equations, the total energy (solid and gas) conservation equation as well as the momentum conservation equation. The latter is pore-averaged to the Forchheimer Law. In addition, MOPAR also takes into account variable coordinate systems (cylindrical and spherical), and allows ablation on both sides of the domain, using a new tri-diagonal solver. The code has been verified and validated, and has been compared to both CMA and FIAT. It also has been strongly coupled to LeMANS, a hypersonic CFD code, to solve integrated problems, ranging from re-entry capsules to kinetic energy penetrators.

The results presented here are part of the inter-code calibration exercise. The values for all of the in-depth temperatures, the surface temperatures and blowing rates agree identically to the reference output obtain with FIAT. It is to be noted that MOPAR solved the momentum equation for the test problem, through Darcy's Law, and FIAT does not. For such a material, with those general simulation conditions, it is clearly not necessary to do so. Finally, the test-case was run at a much finer resolution, both in space and time, than the output provided from FIAT. It is therefore possible to observe, in great detail the first few seconds of the simulation. During this time, the blowing rate peaks at much higher values than the FIAT code predicts, before asymptotically decreasing.

Prediction of Density Degradation of Low Density Material Using the CHALEUR Code

Ben Blackwell, Micah Howard and Dave Kuntz, *Sandia National Laboratories, USA*

The Sandia developed CHALEUR code has been exercised as part of a NASA/Air Force/Sandia code comparison exercise. The material was specified to be a low density thermal protection material that was developed by NASA with properties being available in the open literature. The CHALEUR code is one dimensional with 2nd order spatial discretization and either 1st or 2nd order time integration with Arrhenius decomposition kinetics. The code was exercised both with and without the Darcy flow options. Predictions were made for temperature and solid density as a function of time and results compared favorably with reference results provided by the conference organizers. Because of the specified problem parameters, there was negligible pressure rise inside the material. Consequently, the results with and without Darcy flow were almost identical.

MIG: Results for the Inter-code Calibration Exercise

Ankush Bhatia and Subrata Roy, University of Florida, USA

We are interested in participating in the inter-code calibration and validation exercise in the Fourth Annual AFOSR/NASA/SNL Ablator Modeling Workshop and give an oral presentation on our modeling effort. We are developing a Type II ablation code, i.e. classical thermochemical ablation models with phenomenological in-depth chemistry. It currently has the capability to solve a 1-D thermal ablation problem, and work is being done to extend it to higher dimensions (2-D and 3-D). Numerical scheme employed in the code is time-implicit discontinuous Galerkin (DG) method, which is based on a finite element framework provided by our in-house, Multi-scale Ionized Gas flow code or MIG. The code has been used to solve an arc-jet case, where a test sample, made of carbon phenolic, is exposed to a heat flux value of 1400 W/cm2. The test sample undergoes thermal decomposition at high temperatures, and releases a mixture of gases, or pyrolysis gas. The code solves for thermal response of the material under given external conditions. Material is taken to be porous, and flow of pyrolysis gas through a porous media is considered. Both the Darcy’s friction coefficient and deviation from Darcy’s law are considered to model the flow of pyrolysis gas through porous material. In addition, we also solve for continuity, momentum and energy transport equation for the pyrolysis to correctly account for the net cooling effect provided by the pyrolysis gas as it travels through the ablating system. In our current work, we consider the gas to be at equilibrium at the temperature of the solid material and net pressure of the gas. We have benchmarked our results with the data published by Ahn and Park, and presented them in both 2010 and 2011 AIAA Aerospace Sciences Meeting in Orlando, Florida. We intend to validate our discontinuous Galerkin method with available thermal ablation test data and also broaden the application of our model for general thermal ablation problem through this workshop.

Aerofast: Thermal/Ablation Analysis of the Front Heat Shield for a Martian Aerocapture Mission

A.J. van Eekelen, SAMTECH s.a., Angleur-Liège, Belgium, G. Pinaud & J.-M. Bouilly, ASTRIUM-SAS, St. Médard-en-Jalles, France

An Aerocapture vehicle traveling from Earth to Mars, approaches that planet on an hyperbolic interplanetary trajectory. Upon arrival, the vehicle will perform a single atmospheric pass to significantly reduce its speed, and enters into an orbit around the planet. This maneuver uses aerodynamic drag instead of propulsion for orbit insertion, and potentially leads to large mass (fuel) savings as well as reduced flight times (higher arrival speed). However, Aerocapture results in significant aerodynamic heating, necessitating a Thermal Protection System (TPS), as well as the use of a guidance system to assure that the spacecraft leaves the planetary atmosphere on the correct trajectory.

In the frame of the seventh European Community Framework Program (FP7), the AEROFAST (AERO- capture for Future space tranSporTation) research and development project aims at preparing a demonstration of a Martian Aerocapture mission and increasing the Technology Readiness Level (TRL). The aim of this poster is to present the preliminary thermo-mechanical analysis and design of the front-shield of the space probe. Despite the fact that several probe aerodynamic shapes and concepts are still being evaluated, this poster focuses only on the analysis of a 3.6 m diameter heat-shield, of an Apollo like shape with a low density phenolic impregnated cork as TPS. The 3D heat load history (convective and radiative), over the front-shield, is based on the maximum energy trajectory associated to a constant bank angle of 180◦ in a CO2 Martian atmosphere.

During the first part of the project the implementation and validation of a 3D ablation and charring material model in the finite elements program SAMCEF Amaryllis was achieved. This was done by comparing the results of the 3D and 2D axisymmetric studies, performed on the leeward and the windward side of the probe. The numerical model consists of three sets of equations, namely the transient heat balance equation, the steady state mass balance equation and the charring equations. For the charring of the material we use a multi-species Arrhenius model with the species densities as degrees of freedom. The ablation is modeled by a surface imposed and temperature dependent ablation speed, followed by an in volume mesh deformation.

During the second part, a preliminary design (allowable thickness versus curvilinear abscissa) of the TPS was obtained for the cork based material. The shape and mass evolution, during the Aerocapture phase, provides input for the mass budget and for the guidance and control analysis.

NIDA – A Non-Equilibrium based In-Depth Ablation Code

Gary C. Cheng and Balaji Shankar Venkatachari, University of Alabama at Birmingham, USA

Charring ablative thermal protection system (TPS) has been commonly used to prevent the payload of a hypersonic or space exploration vehicle from exposure to high heat loads. The physical phenomena associated with the pyrolysis of the charring ablative material are very complex, that numerical simulations are needed to supplement the traditional TPS design methods for gaining a better understanding of the process. However, most of the existing state-of-the-art numerical models are built with the assumptions that (i) pyrolysis gases do not interact in-depth with the ablative material and (ii) pyrolysis gases released during the thermal decomposition of the resin phase are in chemical equilibrium. As a result, they fail to account for the heat absorption effect of the flowing pyrolysis gas and also predict the exit gas composition at the ablator surface incorrectly, thereby introducing significant uncertainties in the design process. In an attempt to overcome these drawbacks, a high-fidelity numerical model capable of accurately simulating the behavior of charring ablative TPS has been in development under NASA Constellation University Institutes Project. The NIDA (Non-equilibrium In-Depth Ablation) code is a quasi one-dimensional program that is designed to simulate decomposition of charring ablators and the transport as well as chemical reactions of the associated pyrolysis gas through the char layer as a continuum. Its unique aspect is that it models the transport and the chemical kinetics of pyrolysis gases through the ablator completely. Other features of NIDA include: (i) variable porosity of the char, (ii) temperature-dependent thermodynamic properties of char and pyrolysis gases, (iii) thermal non-equilibrium between the char and the pyrolysis gas mixture, (iv) surface recession, (v) Darcy's law to account for pressure variation, (vi) material decomposition, and (vii) in-depth pyrolysis. In this study we target the calibration of NIDA against existing codes, utilizing the theoretical ablator that has been

A Conservation-Law Form of the CMA In-Depth Ablation Model

Graham V. Candler, University of Minnesota, USA

The Aerotherm CMA code and associated model are the basis for most present in-depth ablation and thermal response analysis methods. In this poster, we re-examine the basic governing equations and recast them in conservation-law form, which is more amenable for use with current computational methods. The basic approximations for the CMA model are retained, and the results are compared to the solution of the CMA form of the equations for the TACOT test problem. The use of a Darcy Law for the pyrolysis gas flow and the assumptions associated with the pyrolysis gas state are also investigated.

Hero: Heat Transfer and Erosion Analysis Program

G Mark E. Ewing, Daron A. Isaac, and H. Heath Dewey, ATK Aerospace Systems, USA

Hero (Heat Transfer and Erosion Analysis Program) is a multi-dimensional thermal ablation code developed by ATK. The program is based on a hierarchic finite-element numerical scheme with a variable grid. Calculations for heat transfer, material pyrolysis, internal pore pressure and thermochemical surface ablation are provided. The program is well-suited for modeling of complex geometries and anisotropic materials. The program also includes capabilities for surface-to-surface radiation exchange as well as structural modeling using the same grid used for thermal solutions. The structural capabilities enhance modeling of thermal-structural interactions and facilitate research related to the thermal-structural response of ablative insulators. The program has been extensively verified for numerical accuracy. Recent enhancements to the program have included error estimation, adaptive discretization and element enrichment, and parallel processing capabilities.

Nonequilibrium Ablation and Pyrolysis: A Fundamental Approach

J. B. Scoggins and H. A. Hassan, North Carolina State University, USA

The Nonequilibrium Ablation and Pyrolysis (NEQAP) code implements a one-dimensional ablation and pyrolysis model derived from first principles for Carbon-Phenolic Thermal Protection Systems. Traditionally, ablation models assume in-depth pyrolysis gases to be in chemical equilibrium as well as in thermal equilibrium with surrounding char material. The goal of NEQAP is to remove these assumptions in order to study the effects they have on current material response predictions including pyrolysis gas composition in-depth and their flux into the boundary layer. The pyrolysis gas densities in-depth are computed by solving species mass conservation equations for a homogeneously reacting ow through a porous medium with the velocities approximated by Darcy's Law. In addition to the mass conservation equations, the char and gas temperatures are treated separately via two energy conservation equations. The temperature inside the virgin layer is computed through a separate energy equation. Due to a lack of heterogeneous kinetic data, the porosity is computed through a temperature curve derived from Thermogravimetric Analysis data for PICA. Surface recession is governed by a detailed energy balance along with the carbon deposition model of Park. The model predicts temperature distribution and pyrolysis gas composition inside the char layer and the composition of their flux into the boundary layer over time. In addition, both m_c and m_g which are the mass removal rates of the surface and phenolic resin respectively, are predicted as part of the solution.

Prediction of Material Decomposition of a Low Density Material Using the CMA Code

Micah Howard, Dave Kuntz and Ben Blackwell, Sandia National Laboratories, USA

The material thermal response code CMA was used as part of a NASA/Air Force/Sandia code comparison exercise. CMA was originally developed by the Aerotherm Corporation in the 1960s and has since been extensively modified and used by Sandia. CMA is a one-dimensional finite difference code that predicts the thermal response of a decomposing material. The material behavior within CMA is based on a three component model with Arrhenius decomposition kinetics. The material used for the comparison exercise is a low-density thermal protection material that was developed by NASA with properties being available in the open literature. Predictions were made for temperature and solid density as a function of time and results compared favorably with reference results provided by the conference organizers.

PATO Results for the 2011 Ablation Test-case

Jean Lachaud, University of California - Santa Cruz, USA and Nagi N. Mansour, NASA Ames Research Center, USA

A Pyrolysis and Ablation Toolbox based on OpenFOAM (PATO) is being developed for academic research purposes. Its purpose is to provide a modular research platform to test high-fidelity models for ablative materials subjected to high enthalpy flow conditions. The OpenFOAM open source CFD software package is used as a framework to produce this modular toolbox. Classes specifically needed to handle the pyrolysis-ablation problem (B' table interpolation, equilibrium solver, etc) have been integrated into the object-oriented structure of OpenFOAM. Governing equations are written in a top-level solver in their mathematical form and may be modified to test new models. This allows the process of equation discretization to be avoided with the relevant finite-volume schemes and solvers being chosen at execution time.
The current suite is composed of 3 modules:

-PAM_1, implementation of the state-of-the-art CMA model;

-PAM_2, 3D solver with a 3D treatment of the pyrolysis gas flow (averaged momentum equation);

-PAM_3, currently in development, will be a high-fidelity module including finite-rate chemistry, multicomponent diffusion, in-depth ablation, and coking.

PATO results for the 2011 ablation test case will be presented in the ablation test-case overview session [5 minutes, 2 slides]. A description of PATO will be detailed in the poster session with a summary of the test case results and an illustration of a 3D case with 3D pyrolysis gas.

Charring Ablator Thermal Response Model (CAT) - a High-Fidelity Material Response Model

J Nagi N. Mansour, NASA Ames Research Center, USA; Jean Lachaud, UARC, University of California -- Santa Cruz, USA and Thierry Magin & Julien de Muelenaere, von Karman Institute, Belgium

Low-density carbon/phenolic is a class of ablative materials that is attractive for blunt body space vehicles where weight and performance of the material are of primary importance, but shape preservation is not critical. Phenolic Impregnated Carbon Ablator (PICA) is of this family. PICA has gained heritage with the success of the Stardust mission. Its performance has been extensively tested in support of the Constellation program and the Mars Science Laboratory (MSL) aeroshell design. PICA-X, also of the same class, has been successfully used on Dragon, the commercial Space-X capsule. Most important for the engineering community, the MSL aeroshell has been instrumented, and extensive flight data for this material is expected in 2011 from the MEDLI project.

Current material response models are inspired from the model of Kendall et al. published in 1968. This model has been able to reproduce within a reasonable accuracy, Arc Jet performance tests carried out on PICA in conditions relevant to NASA's missions. Therefore, depending on the design layout and quantity of interest, current models are robust. In off design conditions, however, there is a strong need to improve current models. In the poster, a high-fidelity model, tailored for PICA family material architecture, is detailed and discussed. The model tracks the chemical composition of the gases produced during pyrolysis. As in the conventional model, it uses equilibrium chemistry to determine the recession rate. It also tracks the time evolution of the porosity of the material. Progress towards implementing this high-fidelity model in a code baptized, CAT, is outlined. Results for the workshop test case are presented as part of the verification process of the code development.

Numerical Rebuilding of Ablative Test Cases using KCMA

Philippe Reynier, Ingénierie et Systèmes Avancés (ISA), France

In the frame of its activities NASA as defined a one dimensional test case for assessing the capabilities of numerical tools dedicated to ablation. The objective of the test case is to compare in-depth ablation physics available in ablation codes. The test case focuses on a pyrolysing material without surface recession.

The current test case will be rebuilt using KCMA which has already been used for the similar efforts carried out in the frame of the European Ablation Working Group for the reconstruction of experimental measurements performed for graphite and carbon phenolic.
KCMA is based on a one dimensional approach and uses a surface energy balance at the material surface. It is based on a finite difference centred scheme accurate to the first order in time and the second order in space is used for solving the equations, and can compute TPS recession for stagnation point and cone configurations (for a dedicated point).

Several balance equations are solved for the gas and solid phases:
-The solid density accounting for pyrolysis;
-The gas density, taking into account pyrolysis, material porosity, changes of gas density under pressure effects, blockage;
-Gas momentum equation;
-Total energy conservation.

Porosity and gas friction within the material can be accounted for. The wall temperature and the mixture composition are calculated using the hypothesis of a wall at chemical equilibrium, and the surface temperature can be also imposed. Species mass fraction, temperature and density in the boundary layer are computed using the method of Gordon & Mc Bride and the data of JANNAF and/or Gurvich for computing the species specific heat, enthalpy and free entropy.

So far different materials can be handled by the tool. Carbonaceous materials, with and without pyrolysis, in this case carbon oxidation and sublimation are considered, while nitridation is not considered. The tool capabilities have been recently extended to silica based materials and melting of silica is taken into account for calculating the recession.

The results provided by the tool have been compared with the results obtained during the Pioneer-Venus mission, and the experimental data available for graphite and carbon phenolic. In the final contribution, numerical results on temperature distribution inside the material and char thickness for the defined test case will be predicted.

Description and Results of a Predictive Model for Pyrolysis

Rochan R. Upadhyay, The University of Texas at Austin, USA

We consider a model for in-depth pyrolysis using a continuum theory of mixtures. The material is assumed to be composed of a number of distinct solid and gas phases. The pyrolysis process is modeled as an inter-conversion of different constituent phases. The gas transport is assumed to be instantaneous and therefore gas momentum equation is not solved. We use data provided for Carbon Phenolic. Results show good (but not exact) agreement with FIAT results. Differences could be attributed to different treatment of the transport properties of the solid mixture and the integration of pyrolysis kinetics.

Computation of the TACOT intercalibration Testcase for the 4th AFOSR/SNL/NASA Ablation Workshop using FABL

Jim Merrifield, Fluid Gravity Engineering Ltd, UK

The TACOT testcase will be computed using FGE's ablation code FABL. Results will be presented for the purposes of inter-model comparison and calibration. FABL is a 'standard' effective properties code with the following modules:

1. Basic numerical method : STAB2 (1D implicit shrinking grid with multi-materials , contact resistances etc)
2. Multiple Arrhenius decomposition from TGA, with arbitrary grouping (resin/fibres/contaminants)
3. Equilibrium or non-equilibrium pyrolysis gas treatment
4. Internal pressures from Darcy type law
5. Iterative TPS sizing for input design rules.
6. Adjoint scheme and simple optimiser for fitting of effective properties to arc heater or flight measurements (or sets of)
7. Simple surface chemistry modules for surface energy balance:
    a. Carbon ablation (kinetic, diffusion limit, sublimation)
    b. Teflon model
    c. Melt failure (silica etc)
    d. Variable surface stoichiometry materials + failure
    e. Surface roughness evolution model based on differential ablation rates, shape factor and Dirling correlation. (used when coupling to flow codes)
8. Flame front model with equilibrium/frozen burn treatment for pyrolysis gases for charring ablators. The burn efficiency is an empirical factor.

Boundary conditions can be defined in terms of temperature or heat flux.

POSTERS

An Inverse Parameter Estimation Methodology for the Analysis of Aeroheating and Thermal Protection System Experimental Data

Milad Mahzari, Ian Clark & Robert Braun, Georgia Institute of Technology, USA and Ioana Cozmuta, ERC Inc., USA

There are substantial uncertainties in the computational models currently used to predict the heating environment of a spacecraft and the Thermal Protection System (TPS) material response during Mars entry. Flight data will help with a better quantification and possible reduction of such uncertainties as well as with the improvement of the current computational tools. The Mars Science Laboratory (MSL) entry, Descent and Landing Instrumentation (MEDLI) suite will provide a comprehensive set of flight data. The Inverse Parameter Estimation (IPE) methodology presented in this work targets the reconstruction of the boundary conditions experienced by the spacecraft during the entry in the Mars atmosphere, in particular the heating to which the TPS is exposed. To investigate the feasibility of the IPE method, Arc Jet test conditions relevant to MSL entry environments are selected. The Nominal Analysis is performed first to examine the quality of the experimental data and to compare to the nominal model predictions. Next, a Monte Carlo study is performed to provide a hierarchy for the model input parameters based on their overall contribution to the measurement uncertainty. A Sensitivity Analysis is then performed where the correlation between the different input parameters is investigated to determine whether they can be simultaneously estimated. Finally, an IPE code is developed and tested on the ArcJet dataset. This code uses in depth temperature information and recession data to back calculate heating and material properties. Solution uniqueness, existence and stability are discussed in detail and are being identified as the main challenges of the inverse analysis.

Carbon-Phenolic-In-Air Chemistry Model for Atmospheric Re-entry

Alexandre Martin, University of Kentucky, USA, Iain D. Boyd, The University of Michigan, USA and Ioana Cozmuta, ERC Inc., USA

Recent and future re-entry vehicle designs use ablative material as the main component of the heat shield of their thermal protection systems. In order to properly predict the behavior of the vehicle, it is imperative to take into account the gases produced by the ablation process when modeling the reacting flow environment. In the case of charring ablators, where an inner resin is pyrolyzed at a relatively low temperature, the composition of the gas expelled in the boundary layer is complex and might lead to thermo-chemical reactions that cannot be captured with simple flow chemistry models. In order to obtain better predictions, a proper gas flow chemistry model needs to be included in the CFD calculations. Recent calculations showed that extensive differences were found in boundary layer composition and heat fluxes, both convective and radiative, when previously published models were used. Recently, a more complete model was proposed, which includes an extensive set of kinetic rates, taken from the combustion community. Using this model, CFD calculations of the Stardust re-entry are presented. The results clearly demonstrate the need to account for many more species in the flow field than the ones that are expected to be present at the surface. The results are then used to obtain non-equilibrium radiation spectral data, which are compared to the experimental data obtained during Stardust re-entry by the *Echelle* instrument.

Modeling of Ablation Using the DSMC Method

Erin D. Farbar and Iain D. Boyd, The University of Michigan, USA

Many of the future materials of interest to NASA for atmospheric re-entry are ablators. When a charring ablator is used, thermal pyrolysis of the heat shield material produces an inner gas which then flows through the surface and into the flow field. Additionally, the exposed surface of the material reacts and eventually looses mass and recesses. At high altitude, the latter phenomenon is not dominant, and the majority of the ablative products come from the inner structure of the material. The pyrolysis process starts early in the re-entry trajectory, often when the vehicle has not yet reached the continuum region. In order to model these types of noncontinuum ablating flow fields, the Direct Simulation Monte Carlo (DSMC) method is used. The DSMC method is a kinetic numerical technique that has been used to simulate gas flows in translational, chemical and thermal nonequilibrium for many applications. The DSMC method involves following a representative group of simulated particles throughout the computational domain, as they move and collide. Individual models are employed to account for physical processes, such as chemical reactions, excitation of internal energy modes and gas-surface interactions. In this work, an existing DSMC code is modified to include the injection of a gas with a specified composition and mass flow rate from the vehicle surface into the flow field. The surface-normal velocity components of the injected particles are sampled from a biased Maxwellian velocity distribution at the specified constant surface temperature. As a first step toward the implementation of a fully reacting surface boundary with blowing, the well documented IRV-2 vehicle test case is used to test the new boundary condition. The free stream conditions at an altitude of 67 km are used, with a vehicle velocity of 6780.6 m/s. The Knudsen number, indicating continuum breakdown, is approximately 0.03 based on the nose radius of the vehicle. This places the 67 km flight condition in the non-continuum flow regime. An isothermal wall temperature of 1600 K is imposed, as is a fixed blowing rate of 0.033 kg/m2/s of CO. The influence of the ablation products on the surface heat flux and shock stand-off distance is investigated. Additionally, the DSMC results are compared to results obtained using the CFD code LeMANS. Qualitative agreement between the two sets of results is observed, however there are significant differences in the predicted CO concentration and flow field temperatures. The latter discrepancy is observed in comparisons of DSMC and CFD flow field results.

Extension of the PECOS Quasi-steady Ablation Toolkit for Uncertainty Propagation

Reed Anzalone, R. Rochan Upadhyay, and O.A. Ezekoye and The University of Texas at Austin, USA

Low-order models are quite useful for sensitivity analysis and design. This work details work done on adding complementary pieces to the PECOS low-order, quasi-steady-state ablation model to facilitate uncertainty propagation. The PECOS quasi-steady state ablation model is a one-dimensional, quasi-steady-state, algebraic ablation model that uses finite-rate surface chemistry and equilibrium pyrolysis-gas-production submodels to predict surface recession rate. The material response model is coupled to a film-transfer boundary layer model to enable the computation of heat and mass transfer from an ablating surface. For comparison to arc jet data, a simple shock heated gas model is coupled. A coupled model consisting of submodels for the shock heated gases, film heat and mass transfer, and material response is exercised against recession rate data for surface and in-depth ablators. Comparisons are made between the quasi-state-state ablation model and the unsteady ablation code, Chaleur, as well as to other computations for a graphite ablator in arcjet facilities. The simple models are found to compare reasonably well to both the experimental results and the other calculations. Uncertainty propagation using a moment based methods is presented. The method is applied to a number of simplified sample problems, for both univariate and multivariate scenarios. The results of this study are discussed, and conclusions about the utility of the method as well as the properties of the ablation code are drawn.

Feasibility of Ablation Measurements in Small Particle Hypervelocity Impact Range Facility

Alina Alexeenko, Marat Kulakhmetov, Mikhail Slipchenko, Steven Schneider, Purdue University, USA and Jonathan Mihaly, Marc Adams, Ares Rosakis, California Institute of Technology, USA

The use of free-flight hypervelocity projectiles for ablation measurements is considered in this work. The California Institute of Technology's Small Particle Hypervelocity Impact Range (SPHIR) features a two-stage light gas gun that launches a 1.8mm projectile with masses between 5-10mg at velocities up to 10 km/s. With the application of modern high-speed high-sensitivity optical detectors, measurements of the exterior ballistics phenomena considered herein can be done with the very high temporal and spatial resolution. The state-of-the-art cameras, spectrometers and trigger/timing circuitry with 1 to 10 ns response time and up to GHz framing rates allows to collect data on crucial thermo-physical parameters including the ablative species concentration, velocities, and temperature which can be extracted to validate and improve existing high-enthalpy flow and ablation models. Direct Simulation Monte Carlo flow and heat transfer calculations are presented for spherical projectiles at conditions typical for the SPHIR facility, e.g., 1 Torr ambient pressure and 5 km/s velocity. The analysis is used to assess the feasibility of reaching significant rates of ablation within the thin outer layer of the projectiles. The threshold levels of ablation products in the shock cap and wake of projectiles are estimated that can be determined from the radiation intensity map in a spectral range away from atomic and molecular peaks.

Experimental Support for Ablation Model Parameter Development and Solid State Thermal Decomposition

David R Payne, Defense Science and Technology Laboratory, UK

To predict the high temperature behavior of a carbon/phenolic charring ablator, a model of the thermal decomposition of resin is required. This model should represent the intrinsic behavior of the resin independent of the experimental conditions. The current method of representation is to use an Arrhenius expression, the apparent kinetic parameters having been obtained from a thermogravimetric analysis (TGA) test. This can simply be described as a curve fitting exercise, without any chemical significance attributable to the calculated apparent kinetic parameters. The scientific community has not, to our knowledge, provided any other method of representation of the kinetics of a reaction in the solid state. Therefore the ablation community continues to make use of this empirical expression. The result is that there is currently no connection between the kinetic parameters used to represent the solid-state thermal decomposition of the resin and the pyrolysis gas chemistry. As well as this, there is limited understanding of the fundamental thermal decomposition reaction mechanism. Succinctly put, the current research goal is to predict a thermogravimetric analysis test (mass loss versus temperature curve, at a given heating rate) under a prescribed set of experimental conditions. This requires understanding of the intrinsic chemical rate of reaction independent of the effects of heat and mass transfer.

The presentation will briefly cover 3 areas:
1) Standard TGA testing of phenolic resin and the interpretation of the decomposition events as a function of heating rate. Current work including high rate tga (up to 500ºC/min) will be compared with previous high rate TGA in the literature.
2) Results of preliminary analytical pyrolysis of phenolic resin to identify the condensable and gaseous, decomposition products.
3) Preliminary molecular dynamics modeling of the thermal decomposition process of phenolic resin using ReaxFF.

It would be useful to discuss the current aspirations of the ablation community as well as the relevance of the approach outlined above.

Experimental Support for Ablation Model Parameter Development and Solid State Thermal Decomposition

Paul Norman and Thomas Schwarztentruber, University of Minnesota, USA

Accurate characterization of the aerothermal heating on vehicles traveling at hypersonic velocities is essential to their design and capabilities. One significant contribution to the heating can come from the heterogeneous recombination of species dissociated in the shock layer on the thermal protection system of the vehicle. The goal of this work is to develop a surface catalysis model for air on SiO2, which is a significant component in both ablative and reusable heat shields. Our initial efforts focus on identifying and describing the mechanisms for the recombination of atomic oxygen on quartz-SiO**2**. These mechanisms can be incorporated into Computational Fluid Dynamics simulations in the form of a Finite Rate Catalytic (FRC) Wall Boundary Condition to accurately describe the chemical reactions and heating on the surface of a vehicle. To accomplish these goals, we perform reactive molecular dynamics simulations using the ReaxFF potential, which naturally allows bond formation and breaking to occur during the course of a molecular dynamics simulation. Silica surfaces are populated with a gas of atomic oxygen at various temperatures and pressures using a flux boundary condition. Once populated, recombination coefficients and the rates of individual reactions can be measured by counting events. The measured recombination coefficients have an exponential trend with temperature, with an activation energy in reasonable agreement with experimental results. These simulations are used to identify several possible pathways for recombination, which include the Eley-Rideal and Langmuir Hinshelwood mechanisms. Individual reaction rates from the FRC model are then investigated using single-collision molecular dynamics simulations.

Catalysis and Oxidation of Copper Calorimeters – Are we Over-Testing Material Samples?

Jose Santos and Anuscheh Nawaz, Sierra Lobo Inc, USA

Arc-jet tests are the most important criteria for designing and accepting thermal protection systems (TPS). Their plasma plume is characterized by using a copper calorimeter measuring heat flux, which is inserted into the stream. The measured heat flux value is then converted to incident hot wall heat flux at which a thermal protection material is tested. The model assumptions used to convert the calorimeter reading to an equivalent hot wall heat flux are currently based on the assumption of full catalycity of copper during plasma exposure, meaning that the plasma chemical energy is fully converted to heat flux. Oxidation effects on the copper calorimeter and on the heat flux are not considered - despite the fact that it is expected of copper exposed to air plasma to change surface composition and morphology. Literature shows that different copper oxides form at different temperatures; each of them being characterized by a lower catalytic coefficient than that of pure copper. The value of the heat flux at which TPS are currently tested is thus higher than required, leading to over-dimensioning the TPS for a flight design. An effort is needed, which aims at providing a clear understanding of the oxidation effects on copper calorimeters exposed to various arc-jet test conditions and the direct impact oxidation has on the resulting catalytic coefficient. This would enable us to correct the models and thus test TPS under more accurate aero-thermal environment. This will ultimately lead to more realistic TPS weight budget for all EDL missions (in particular where high enthalpies are expected during entry such as into Earth and Mars), increasing mission payloads and moving into reach missions that currently, from a TPS perspective, seem impossible. The proposed poster will highlight unknown areas of error when using copper calorimeters for heat flux characterization. It will propose a path forward, and serve as a baseline for discussion and potential collaboration.

Ablation and Drag Modeling for Reentry of a Blunt Body with Complex Geometry Maria Gritsevich

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An analytical modeling to describe hypersonic movement of a blunt body in an atmosphere is considered. The body is taken to be of unknown shape with complex geometry. We permit further changes in the body shape during the whole luminous part of an atmospheric trajectory. Using the basic differential equations one can introduce the dimensionless parameters describing a problem. Then the study takes an approach that models the body's mass and other properties based on the height and rate of body deceleration in an atmosphere, which also provides us a good link for better understanding accompanying radiation processes. The model is fitting to the actual data of observations, by selecting key dimensionless parameters describing drag, ablation and rotation rate of a body. The obtained parameters explicitly characterize the ability of entering body to survive an atmospheric entry and reach the ground.

Modeling of Crack Propagation in AVCOAT, a Charring Ablator

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Objective of this work is to estimate the potential growth of a tapered crack on an AVCOAT ablative TPS in the arcjet environment and in flight. To accomplish this objective, we have developed a simple one-dimensional model of pyrolysis blowing rates for AVCOAT which allowed us to determine the maximum chemical ablation rate in the arcjet and along a reentry trajectory. The research was done in four stages. First solutions of the arcjet flow over a crack specimen were obtained. In addition, flow solutions over the CEV module for a range of altitudes, varying from 100 to 70 km were performed. From these simulations, the heat flux was estimated at the stagnation point/crack inlet and the AVCOAT material thermal response was calculated to estimate the pyrolysis gas flow rate emitted by the walls of a tapered crack tile. Finally the interaction of the boundary layer gases in the crack channel with the pyrolysis gases was studied. Chemical ablation along the channel surface was computed at various altitudes.