5th Ablation Workshop

February 28th - March 1st 2012
Hilton Lexington/Downtown, Lexington, Kentucky
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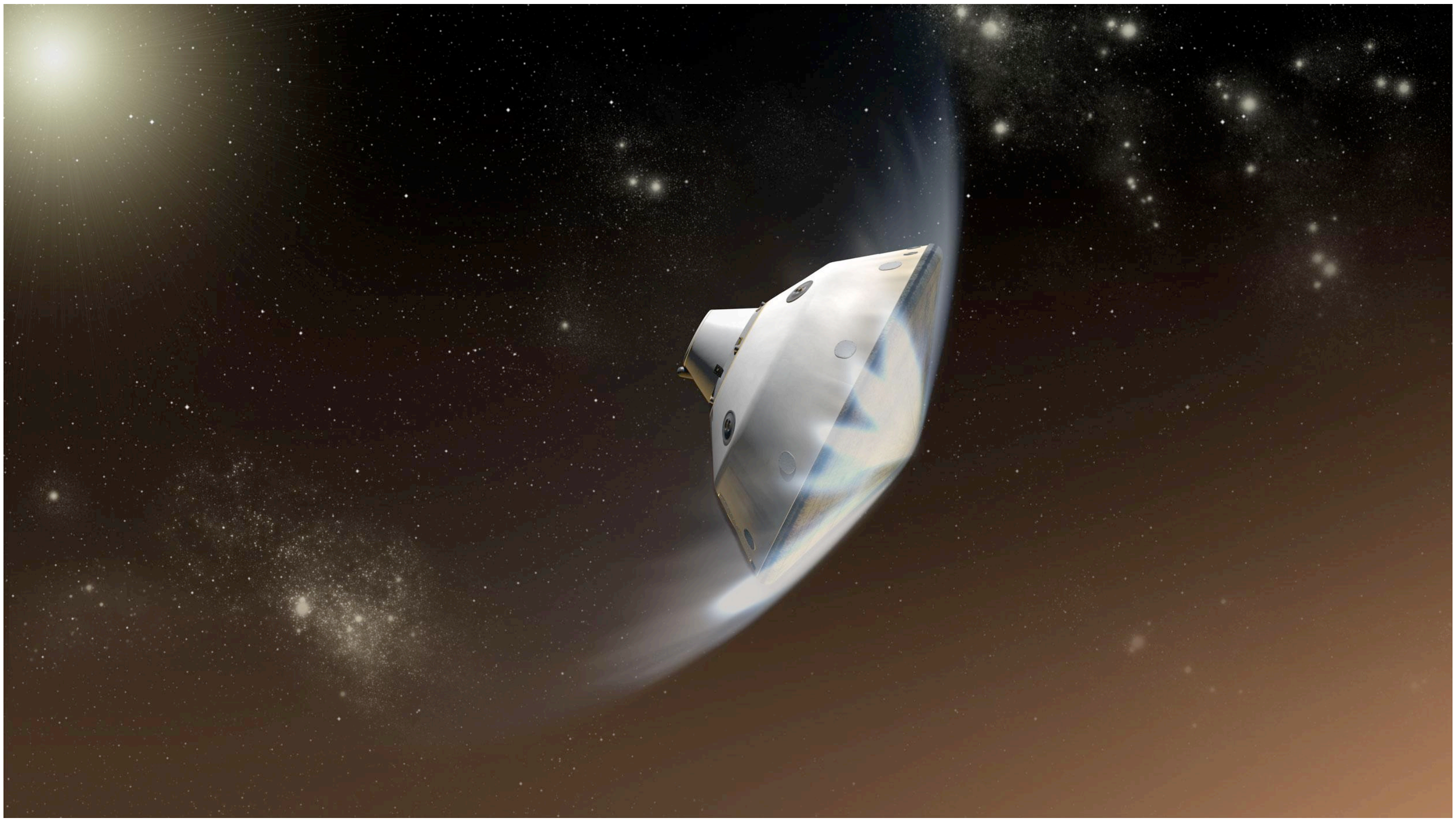
University of Kentucky



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Proceedings of the 5th Ablation Workshop

Edited by

Alexandre Martin, University of Kentucky
Ioana Cozmuta, STC Inc / NASA Ames Research Center

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Lexington, Kentucky

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Welcome to Kentucky!

The Local Organizing Committee is very happy to welcome all attendees to the 5th Ablation Workshop, in Lexington, Kentucky. Steered by NASA, Sandia National Labs and the Air Force Office of Scientific Research (AFOSR), the workshop provides an annual meeting point for all researchers working in the area of re-entry ablation. For the first time, the workshop is being hosted by an academic institution, namely, the University of Kentucky.

Located at the heart of Kentucky, Lexington offers the charm of a small city combined with the soul of a college town. The downtown location of the workshop will surely provide you with an opportunity to fully enjoy the Bluegrass state. Make sure that you savor the very distinct taste of Kentucky's food, and that you don't leave without having tried some fried chicken, a derby pie or the famous *Hot Brown*. Visiting the local bars will certainly provide an opportunity for you to experience the rich musical heritage of the region through live Bluegrass music. And, if you are lucky, you might get a chance to to watch the # 1 ranked University of Kentucky Wildcats NCAA mens basketball team play at Rupp Arena, minutes away from the hotel!

Hopefully you will get a chance to wander outside of the city, into the *rolling hills of Kentucky*. There, you will be able to see the miles of white fences surrounding famous horse farms which breed the finest Thoroughbred horses in the world. Through the off-site activity, you will have the opportunity to experience one of Kentucky's most renowned products, Bourbon whiskey. On top of being able to taste different flavors of Bourbon, you are also invited to tour the Buffalo Trace distillery. The well versed guides will certainly be able to answer all your questions about the nature, production and specifics of Bourbon!

Finally, the Local Organizing Committee would like to thank the sponsors who are making this workshop possible: NASA Kentucky, who provided the majority of the funding, ASTRIUM (France), the Office of the Vice President Research, the College of Engineering and the Department of Mechanical Engineering at the University of Kentucky, as well as NASA's Office of the Chief Technologist, who provided scholarships to students.

As with previous years, the Scientific Committee was able to gather an impressive lineup of speakers; combined with the charm of Lexington, this workshop will certainly be the best yet!

Dr. Alexandre Martin, Chair of the Local Organizing Committee

Foreword

We, the scientific committee, are very pleased to welcome you to the 5^{th} Ablation Workshop in Lexington, Kentucky. Many thanks to the University of Kentucky and Prof. Alexandre Martin, head of the Local Organizing Committee, for his initiative and active fundraising to ensure continuation of this workshop in such a picturesque venue!

The Ablation Workshops, steered by NASA, AFOSR and Sandia, provide a single meeting point for the integration and advancement of a multi-disciplinary research community of scientists and engineers working on aerothermodynamic ablation. This growing research community has members representing government agencies, the private sector, and university systems across the world. The primary objectives of the workshop are to: (1) foster improved communication across international boundaries; (2) expose the aerothermodynamic ablation modeling community to new ideas and techniques from adjacent disciplines; (3) bring new experimental techniques to bear on the problem; and (4) discuss challenges faced in adapting existing techniques to address new applications.

This workshop will take a break in 2013, but for a good cause. The proposal submitted by Dr. Cozmuta to the Gordon Research Council to initiate a Gordon Research Conference in the area of "Atmospheric Reentry Physics" was approved by the board and the first conference will take place February 3rd-8th of 2013 in Ventura, California. This is a great opportunity that ensures continuity for the community to meet and discuss technical topics of high interest in this area. We anticipate that the Ablation Workshop will return in 2014.

Thank you for coming! Please participate, learn something, and above all, have fun!

Dr. John Schmisseur, Air Force Office of Scientific Research
Dr. Michael Wright, NASA Ames Research Center
Dr. Jeff Payne, Sandia National Laboratories
Dr. Ioana Cozmuta, STC/NASA Ames Research Center

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INTRODUCTION: THE 5TH ABLATION WORKSHOP AND BEYOND

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What are the main characteristics of a workshop and what distinguishes a successful meeting from the less successful? It is a simple answer yet very subtle: that of bringing a philosophy to life. Reaching out, encouraging people to participate, get them motivated and involved and strive to make it a permanence and not only a once a year occurrence. That is the real engine behind success.

This year's workshop will focus on the development, validation and uncertainty quantification of the high-fidelity models used to simulate the behavior of ablative materials. Sessions and comparison activities will be held on the various aspects of modeling the surface and in-depth performance of ablative materials, experimental techniques to validate the resulting models, and uncertainty quantification methodologies. The state of the art of ablation modeling has changed little in the past 40 years, largely because of a lack of validation data with which to justify improvements to the baseline models. However, in recent years significant progress has been made on the numerical side, and it is now time to develop a set of validation experiments to test key aspects of the new and proposed models, quantify remaining uncertainties, and prioritize limited research budgets on those aspects that will have the largest impact on minimizing mass and maximizing reliability of spacecraft thermal protection systems.

Beyond the technical aspects, we are committed to make this and every workshop a successful event. To foster improved communication we have reached outside of the traditional community from which this workshop has emerged and we have created a new, broader and more diverse, international community. That has also brought with it an infusion of new ideas, know-how and techniques from adjacent disciplines.

We try our best to make this workshop a dynamic environment, a place where people come to brainstorm about existing problems or simply come up with new ideas that need to be formulated into an innovation challenge. We are not only a simple "problem solving community". We encourage collaboration and combination of ideas in order to maximize the creative potential. And hopefully for ideas identified as being potential innovations to move towards implementation, testing and development. Reviewing the implementation of new ideas should indicate new needs which can be transformed into challenges which, in turn, start a new innovation process cycle and hopefully inspire and change corporate goals and structures. Innovation is the way to keep us continuously challenged.

We tried to create prototypes, such as the theoretical ablator, which are an excellent means for testing ideas. Not only do they allow us to see how an idea would actually look in implementation, but building and playing with a prototype is a good method for further improving upon the core idea. Creating TACOT has given modelers the opportunity to compare the results of their codes. This year we challenge the community with a dedicated session to discuss the setup of an experimental test case.

We work hard to ensure that funding of this workshop and the next ones to come is not an impediment, therefore ensuring that we can keep the community going and growing. 2013 will be the first year of a Gordon Research Conference on the topic of Atmospheric Reentry Physics. Save the date: February 3-8, 2013 in Ventura California! At the workshop we will provide you with key details and requirements specific to a Gordon Research Conference, a tentative technical agenda and a description of the acceptance process for contributions to the conference. For more information please check the Gordon Research Conference website: `http://www.grc.org/programs.aspx?year=2013&program=atmosentry`

Finally, we try to provide the opportunity for you to stay active and involved in-between workshops as well. We encourage you to find and define your level of involvement, commitment and participation. We try to motivate and infuse you with enthusiasm. The discussion times and brainstorming sessions we have allocated in the program serve this exact purpose: to hear your views and ideas. Please come prepared as such!

MERGING AEROTHERMODYNAMIC AND HIGH-TEMPERATURE MATERIALS RESEARCH: AN AFOSR PERSPECTIVE

John D. Schmisseur

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This presentation will provide an Air Force perspective on the current national plans for hypersonic technologies, as well as scientific challenges and opportunities in the disciplines that contribute to the development of hypersonic systems. Additionally, programmatic directions in the portfolios that support research in reentry physics will be discussed.

ABLATION MODELING AND SIMULATION AT SANDIA NATIONAL LABORATORIES

Micah Howard, Ben F. Blackwell, David W. Kuntz and Roy E. Hogan

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This talk will overview ablation modeling and simulation at Sandia National Laboratories, past, present and future. A historical view of ablation simulation capabilities will be presented, followed by a discussion of current work being done to advance our predictive capabilities for ablation problems. Ongoing efforts involve the development of an ablation thermochemistry code, which is being used to solve the thermochemistry problem on-the-fly, hence offering an efficient and more accurate by-pass to traditional interpolation of pre-computed tabular ablation data. This capability has been coupled to Chaleur, a Sandia developed 1D ablation code. Development of a 3D, finite element based ablation code that leverages the ablation thermochemistry code is also underway. This new ablation code involves the investigation of porous flow models and robust mesh motion techniques. Future objectives of this work involve coupling these ablation capabilities with a reacting flow CFD code.

PREPARING NASA FOR THE 21ST CENTURY: OCT PERSPECTIVE ON EDL

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NASA's Chief Technologist, within the Office of the Chief Technologist (OCT), is the principal advisor to the NASA Administrator in matters related to Agency-wide technology policy and programs and is responsible for the planning, advocacy and coordination of technology development activities within NASA to meet future mission needs. OCT works with the Mission Directorates and mission planners to infuse new technologies into future missions and with other Governmental Agencies to coordinate technology development efforts of mutual interest. In addition, OCT manages NASA's Space Technology Program (STP), which also includes the SBIR and STTR programs. In this presentation OCT's role within NASA; the organization of STP; and OCT's investments in EDL will be discussed. These STP EDL related activities range from low TRL to flight demonstration, with a clear infusion path to future Agency needs.

SPRITE: A TPS TEST BED FOR GROUND AND FLIGHT

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Engineers in the Entry Systems and Technology Division at NASA Ames Research Center developed a fully instrumented, small atmospheric entry probe called SPRITE (**S**mall **P**robe **R**eentry **I**nvestigation for **T**PS **E**ngineering). SPRITE, conceived as a flight test bed for thermal protection materials, was tested at full scale in an arc-jet facility so that the aerothermal environments the probe experiences over portions of its flight trajectory and in the arc-jet are similar. This ground-to-flight traceability enhances the ability of mission designers to evaluate margins needed in the design of thermal protection systems (TPS) of larger scale atmospheric entry vehicles.

SPRITE is a 14-inch diameter, 45° sphere-cone with a conical aftbody and designed for testing in the NASA Ames Aerodynamic Heating Facility (AHF). The probe is a two-part aluminum shell with PICA (phenolic impregnated carbon ablator) bonded on the forebody and LI-2200 (Shuttle tile material) bonded to the aftbody. Plugs with embedded thermocouples, similar to those installed in the heat shield of the Mars Science Laboratory (MSL), and a number of distributed sensors are integrated into the design. The data from these sensors are fed to an innovative, custom-designed data acquisition system also integrated with the test article.

Two identical SPRITE models were built and successfully tested in late 2010-early 2011, and the concept is currently being modified to enable testing of conformable and/or flexible materials.

Figure 1: SPRITE model prior to testing in a plasma flow

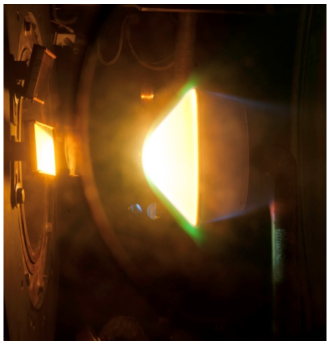

Figure 2: SPRITE model in a plasma flow

Figure 3: SPRITE model after exposure to plasma flow

CHARACTERIZATION OF MATERIAL RESPONSE DURING ARC-JET TESTING WITH OPTICAL METHODS – STATUS AND PERSPECTIVES

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The characterization of ablation and recession of heat shield materials during arc jet testing is an important step towards understanding the governing processes during these tests and therefore for a successful extrapolation of ground test data to flight. The behavior of ablative heat shield materials in a ground-based arc jet facility is usually monitored through measurement of temperature distributions (across the surface and in-depth), and through measurement of the final surface recession [1, 2]. These measurements are then used to calibrate/validate materials thermal response codes, which have mathematical models with reasonably good fidelity to the physics and chemistry of ablation, and codes thus calibrated are used for predicting material behavior in flight environments. However, these thermal measurements only indirectly characterize the pyrolysis processes within an ablative material; pyrolysis is the main effect during ablation. Quantification of pyrolysis chemistry would therefore provide more definitive and useful data for validation of the material response codes. Information of the chemical products of ablation, to various levels of detail, can be obtained using optical methods. Suitable optical methods to measure the shape and composition of these layers (with emphasis on the blowing layer) during arc jet testing are: 1) optical emission spectroscopy (OES); 2) filtered imaging; 3) laser induced fluorescence (LIF); and 4) absorption spectroscopy.

Several attempts have been made to optically measure the material response of ablative materials during arc-jet testing [3, 4]. Most recently, NH and OH have been identified in the boundary layer of a PICA ablator [5]. These species are suitable candidates for a detection through PLIF [6] which would enable a spatially- resolved characterization of the blowing layer in terms of both its shape and composition. The recent emission spectroscopy data will be presented and future experiments for a qualitative and quantitative characterization of the material response of ablative materials during arc-jet testing will be discussed.

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[6] Ben-Yakar, A. and Hanson, R.K., "Hypervelocity combustion studies using simultaneous OH-PLIF and Schlieren imaging in an expansion tube," AIAA99-2453, *35th AIAA Joint Propulsion Conference*, Albuquerque, NM, June 15-18, 1998.

DIRECT OBSERVATION OF MECHANICAL ABLATION

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This presentation describes an experiment that solved a mysterious problem affecting the material that protects solid rocket motor cases from burning propellant gases: Why was the ablation of this material in the forward dome region of recovered flight test motors as much as 2x that observed in full-scale ground test firings?

Heat transfer to the forward dome elastomeric insulation is predominantly radiation from the burning propellant. The 15-kW CO_2 laser at the Wright Patterson AFB Laser Hardened Material Evaluation Laboratory (LHMEL) was used to provide uniform incident radiation from 200 to 400 W/cm^2. We suspected that the rocket acceleration force (which isn't simulated in static firing tests) was removing char layers, so we used a centrifuge to simulate these forces. Gold-plated mirrors directed the laser beam from the centrifuge centerline onto the outward-facing material specimen mounted on the rotating arm. A pyrometer and video camera were also mounted on the arm to observe the specimen response. Accelerations of 0 to 20 gs were generated by varying the centrifuge RPM, and the specimen velocity provided a rudimentary simulation of the convective environment.

The highlight of this presentation is a video that very clearly shows char layers being removed by acceleration forces. At zero and very low acceleration levels, the char layer is robust. At higher acceleration, char layers sequentially grow and are then pulled off when their mass x acceleration exceeds their tensile strength x area. The removal frequency increases with acceleration and heat flux, and some materials are more susceptible than others. The pyrometer data shows a saw-tooth pattern with abrupt surface temperature decreases when char layers are removed to expose virgin material.

This phenomena was modeled using the CMA code modified to include effects of acceleration forces, pyrolysis gas porous flow forces, and char strength. Predictions were consistent with experimental data when an appropriate char strength was input, but of course this was essentially a fudge factor since its impractical to directly measure the tensile strength of an ablating char.

THE MYSTERIES OF REAL MATERIALS

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The presentation will consist in showing arc jet data mysterious to the modelers. It will show a short movie (10-20 sec) of an arc jet test where a material exhibited a failure mode that nobody understands followed by thermocouple data from arc jet tests on another material of interest in which the T/Cs exhibit repeatable, consistent, fascinating yet frustrating response characteristics that have the modelers stumped. This all happens between RT and 200 F. Doesnt sound important? Unless we figure out what it is and can model it, we can't size the TPS with any confidence.

KEYNOTE PRESENTATION – A PERSPECTIVE ON THE DESIGN AND DEVELOPMENT OF THE SPACEX DRAGON SPACECRAFT HEATSHIELD

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Figure 1: Recovered Dragon Spacecraft

In December, 2010, Space Exploration Technologies (SpaceX) successfully orbited, re-entered and recovered their Dragon spacecraft, on an almost "picture perfect" first full mission. Earlier in 2009, SpaceX, announced the passing of a significant technical milestone with the successful arc jet testing of a their new high performance heat shield material, called PICA-X, which provided the primary (forebody) thermal protection for Dragon.

In 2008 and 2009, Dr. Rasky worked closely with SpaceX on the Dragon heatshield design and also developing the ability to manufacture PICA-X. The "X" stands for the SpaceX-developed variants that have several improved properties and greater ease of manufacture than the original PICA used on Stardust. Dr. Rasky will discuss and describe a number of his perspectives and observations from his experience working with SpaceX, including some of the stark contrasts from his 20 years working at NASA.

1. SPEAKER BIO

Dr. Dan Rasky, a Senior Scientist at NASA Ames co-invented PICA (Phenolic Impregnated Carbon Ablator) a rigid, lightweight heatshield that enable the NASA Stardust mission and was adopted by SpaceX for Dragon. The Stardust mission collected samples from the comet 81P/Wild-2 and returned them safely to earth in January 2006, setting the world record for the fastest entry ever of a man-made object at earth at 12.9 km/sec. For his work, Dr. Rasky was selected as a recipient of the NASA Inventor of the Year award for 2007.

ABLATION TEST-CASE SERIES #2

NUMERICAL SIMULATION OF ABLATIVE-MATERIAL RESPONSE: CODE AND MODEL COMPARISONS

VERSION 2.8, FEBRUARY 6, 2012

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1. PREAMBLE

This test-case series on the numerical simulation of the response of ablative-materials really started out of pure curiosity. Code developers and users were curious to see ”how the codes compare” and ”what is the effect of the different hypotheses in the models implemented”. The objective of these test-case series is to propose problems of increasing complexity until it is agreed that the most-elaborated well-defined problem is formulated. The first test-case was mostly a simple heat transfer problem chosen for it’s simplicity (it is summarized in section 2.1). The second test-case series goes one step further, with the objective of reaching the state-of-the-art design level. It will require the patience of the industrial participants for whom this second series will still mean ”running a basic case”, with codes that have already been tested, verified, and validated. It will also require the comprehension of the academic participants for whom it will imply implementing in their codes engineering models, with maybe no other intents than ”running the second ablation test-case series” and comparing their codes with design tools.

2. INTRODUCTION

2.1. Summary of the first test-case

The first test case was defined for the 4th *Ablation Workshop, 1-3 March 2011, Albuquerque, New Mexico* [1]. It was a one-dimensional test case focusing on the in-depth material response - fixed surface temperature and no recession. There were 14 participants (estimated to be about 50% of the community [2]). Three types of material-response codes have been identified:

- Type 1: based on the CMA[3] model or any mathematically equivalent model (heat transfer, pyrolysis, simplified mass transport);
- Type 2: CMA-type + Averaged momentum equation for the transport of the pyrolysis gases;
- Type 3: Higher fidelity codes (chemical/thermal non-equilibrium, etc).

The results had been provided by the participants before the workshop and a summary was presented during the workshop [4]. For type 1 and type 2 codes, differences in the temperature prediction were mostly below 1%. The participants tentatively attributed the differences to slight model differences and implementation and numerical integration errors needing further detailed investigation. The material properties have been interpreted differently by a few participants leading to differences larger than 1%. Codes of type 3 have shown differences and discrepancies that will need further analysis. We propose to thoroughly analyze the first and second test-case series results together at the 5th *Ablation Workshop, Feb. 28- March 1, 2012, Lexington, Kentucky (tentative dates).*

2.2. Introduction of the second test-case series

The purpose of this document is to define the second test-case series aiming at pushing the comparison further and reaching the state-of-the-art TPS-design level. For consistency with test-case #1 and to limit time-investment, most of the parameters and boundary conditions are unchanged. The main modifications will be to: (1) switch from the fixed surface-temperature boundary condition to a convective boundary condition, and (2) introduce surface recession. Computing the ablation rate to obtain the amount of surface recession is a complicated and still open problem. A traditional B' table will be provided to facilitate the in-depth material-response comparison but other tables/methods may be used. A specific test-case dedicated to the estimation of the ablation rate is also proposed. Therefore, the test-case series #2 includes three traditional ablation tests and one additional test dedicated to the estimation of the ablation rate:

- 2.1: low heating, no recession (targeted surface temperature of about 1644 K, cf. test-case 1) - non-physical intermediate case without recession in preparation for 2.2.
- 2.2: low heating (same as test case 2.1), recession
- 2.3: high heating, recession (targeted surface temperature of about 3000 K)
- 2.4: computation of the ablation rate of TACOT for a temperature range of 300K-4000K and an air pressure of 101325 Pa (1 atm). The B'-table format will be used to enable visual comparison.

3. DESCRIPTION OF THE SECOND TEST-CASE SERIES

3.1. Convective boundary-condition test-cases: 2.1, 2.2, and 2.3

The 1D geometry and the theoretical material TACOT of series 1 are re-used. A 1D sample of TACOT of 5 cm is heated on one side for 1 minute (convective boundary condition) at atmospheric pressure with adiabatic boundary condition on the other side. When the heat flux is applied or removed, transitions of 0.1 s (linear ramping) are applied (see figure 1). We will also model the cool-down for 1 minute under the hypothesis that it is a pure radiative cooling.

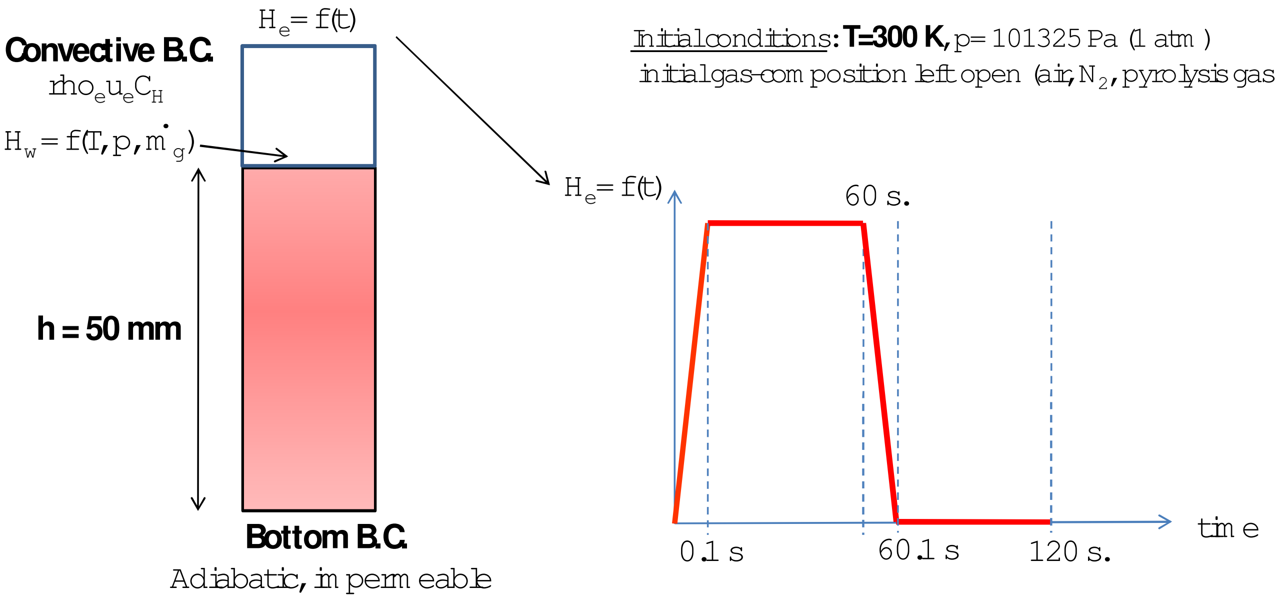

Figure 1: Schematic illustration of the boundary conditions for test-cases 2.1, 2.2, and 2.3

The time-dependent boundary-layer properties are given in table 1.

N.B.: References [3, 5, 6, 2] describing the convective boundary-condition may be obtained from the authors.

Table 1: Summary of the environment properties. Please use linear interpolation during the 0.1s heating and cooling periods (linear ramping).

time (s)	$\rho_e u_e C_H$ ($kg \cdot m^{-2} \cdot s^{-1}$)	h_e ($J \cdot kg^{-1}$)	p_w (Pa)
0	0	0	101325
0.1	0.3	#2.1 & #2.2 : $1.5 \cdot 10^6$ / #2.3: $2.5 \cdot 10^7$	101325
60	0.3	#2.1 & #2.2 : $1.5 \cdot 10^6$ / #2.3: $2.5 \cdot 10^7$	101325
60.1	0	0	101325
120	0	0	101325

The initial conditions are: $p_0 = 1$ atm (101325 Pa), $T_0 = 300$ K, sample length: $L_0 = 0.05$ m. The initial gas composition in the material is left open. For type 1 and 2 codes, pyrolysis gas in thermal equilibrium is the usual practice. For type 3 codes, it is suggested to start with air. The time-dependent boundary-layer properties are summarized in table 1. The other boundary-layer assumptions/properties are as follows for the code comparison:

- The factor for the blowing-correction correlation used is the CMA model is taken as $\lambda = 0.5$.
- Heat and mass transfer assumptions in the boundary layer: $Pr = Le = 1$
- Re-radiation is active during the entire analysis [$q_r = \varepsilon\sigma(T_w^4 - T_\infty^4)$]. Since it is a 1D case, a view factor of 1 is used. The infinity temperature is chosen to be $T_\infty = 300$ K .

Important notes on the recession rate and on the wall enthalpy:

- 2.1: Please read the wall enthalpy (h_w) from the B' table provided in the TACOT_2.2.xls spreadsheet for code comparison and set recession to zero (i.e. $B'c = 0$). Please use an equivalent method if you do not use B' tables. The objective of this test case is to prepare as much as possible for 2.2 but without recession, to avoid mixing boundary-condition and mesh-motion issues during the comparison. It should be outlined that this case is not really physical as the actual wall enthalpy without recession is not equal to the wall enthalpy with recession (different content in carbon in the gas phase). However, it was agreed that this ”numerical” test-case is important for code comparison in preparation of 2.2.
- 2.2: Please use the B'c table provided in the TACOT_2.2.xls file for code comparison or other methods for model comparison.
- 2.3: Idem.

3.2. Ablation-rate test-case: 2.4

The goal of this test-case 2.4 is to compare codes and methods used to compute the ablation rate of the material TACOT. To keep the work load reasonable, we will focus on the following conditions: p= 1 atm; T=300-4000K; under air. B' table (or methods using the same theory) are commonly used - please refer to the literature for definition of B' and B' tables [3, 2, 7]. In this test-case 2.4, we propose two levels of comparison: 2.4.1 and 2.4.2.

- 2.4.1: The first level of comparison consists in comparing B'-table generation algorithms using the following constraints:
  - Air (in mol fractions): O2=0.21, N2=0.79
  - Pyrolysis gas (in mol fractions): C=0.206 / H=0.679 / O=0.115
  - Equal diffusion coefficients, frozen chemistry in the boundary layer, no erosion/failure, CEA database (please use the last version of the CEA2 thermodynamics table: cea092004.inp).
  - Mixture (25 species): C; H; O; N; CH4; CN; CO; CO2; C2; C2H; C2H2,acetylene; C3; C4; C4H2,butadiyne; C5; HCN; H2; H2O; N2; CH2OH; CNN; CNC; CNCOCN; C6H6; HNC.
- 2.4.2: For the second level of comparison, which is more a model comparison than a code comparison, we propose to fix only the following parameters:

  - Air (in mol fractions): O2=0.21, N2=0.79
  - Pyrolysis gas (in mol fractions): C=0.206 / H=0.679 / O=0.115 (species may be used for finite-rate chemistry)

  In other words, for the second level of comparison, the database is open (CEA, JANAF, etc), the boundary layer conditions are open, finite-rate chemistry may be used, etc...

For visual comparison, the usual B'-table plots (B'c= f(T, B'g)) should be used for both 2.4.1 and 2.4.2 if possible. To keep the data load reasonable, we suggest focus on the following conditions: p= 1 atm; T=300-4000K. An example of plot is presented in figure 2. The B' table using the CEA database and a reduced set of 25 species is included in the spreadsheet TACOT_2.2.xls. To enable comparison, we suggest to use the B'g values of the spreadsheet.

4. MATERIAL DATA

The material properties for this test-case series are provided and explained in the spreadsheet TACOT_2.2.xls. Recent updates:

- B' table updated (July 28, 2011)
- Equilibrium properties of the pyrolysis gases up to 4000K (June 2011)

5. CODE OUTPUT AND COMPARISON OF THE RESULTS

An output frequency of $0.1\,s$ will be used for file exchange. Two types of data are required for comparison of the results:

- Type1: temperature response.

  It was found more convenient to use probed values (thermocouples) than temperature profiles. The probed values locations from the initial top surface are: $x_1(t) = x_w(t)$: moving top surface (i.e.,x_1 follows the surface if recession); $x_2 = 1$; $x_3 = 2$; $x_4 = 4$; $x_5 = 8$; $x_6 = 12$; $x_7 = 16$; $x_8 = 24$; $x_9 = 50\,mm$ (x_9 is the bottom surface). $T_1 = T_w$ can be seen as a pyrometer measurement and $T_2, T_3, ..., T_9$ as fixed thermocouples.

- Type2: pyrolysis and ablation response (blowing rates, recession, pyrolysis zone)
  - Blowing rates: we suggest to plot $\dot{m}_g(x = x_w)$ (value at the top surface) and $\dot{m}_c$
  - Pyrolysis zone: we will use again (as in the first test case) the following quantities: virgin 98 % and char 2 % to estimate the location of the pyrolysis and char fronts. The thresholds are defined as: $\rho_v(98\%) = \rho_c + 0.98(\rho_v - \rho_c)$; $\rho_c(2\%) = \rho_c + 0.02(\rho_v - \rho_c)$. For simplicity of the analysis, we suggest to ouput these quantities with respect to the initial top surface.
  - Recession: we suggest to plot the location of the receding surface with respect to the initial top surface (i.e., total recession $= 50 - x_w$)

Output format desired (for analysis by the Thermal Performance Database (TPDB) team)

time (s)	Tw (K)	T2 (K)	T3 (K)	T4 (K)	T5 (K)	T6 (K)	T7 (K)	...
0	3.000e3	3.000e3	3.000e3	3.000e3	3.000e3	3.000e3	3.000e3	...
0.1	9.651e3	3.225e3	3.000e3	3.000e3	3.000e3	3.000e3	3.000e3	...
0.2	1.076e3	3.956e3	3.039e3	3.000e3	3.000e3	3.000e3	3.000e3	...
etc.	...	...	...	...	...	...	...	

Table 2: Output format for the temperature file - please name it: CodeName_Energy_TestCase_2.1.txt

6. PRELIMINARY RESULTS

It has been decided to use CMA as a baseline for visual comparison for test cases 2.1, 2.2, and 2.3. CMA results will be provided by October 2011. In the meantime, **preliminary** results are provided in the following figures. Please do not give them more credit than they deserve and use them for sanity check rather than for comparison.

time (s)	m_dot_g (kg/m2/s)	m_dot_c (kg/m2/s)	Virgin 98%	Char 2%	recession (m)
0	0	0	0	0	0
0.1	5.063e-3	0	0	0	0
0.2	1.340e-2	0	1.781e-4	2.130e-5	0
etc.	...	...	...	...	...

Table 3: Output format for the pyrolysis and ablation-response file - Please name it: CodeName_Mass_TestCase_2.1.txt

7. ACKNOWLEDGMENTS

The test-case definition and the material database have been tested using several codes and will now remain unchanged for this second test-case series. We would like to thank you in advance for any comment that will help to improve the clarity of this document. Please send your comments to the authors. The authors would like to thank: Julien de Mueleneare (VKI) for generating the TACOT_2.2 B' table and proposing the reduced set of 25 species; Jonathan Wiebenga (University of Michigan) for testing the test-cases using MOPAR; Bennie Blackwell (Blackwell Consulting) and Micah Howard (SANDIA) for constructive discussions on B' table generation; Bernie Laub (NASA Ames) for his comments on test-case 2.1. that helped clarifying (hopefully) its very limited scope; Jean-Marc Dupillier (EADS Astrium) for his numerous constructive comments on the TACOT database and on the test-case series.

8. REFERENCES

[1] Lachaud, J., Martin, A., Cozmuta, I., and Laub, B., "Ablation workshop test case - Version 1.1 - Feb. 2, 2011," Prepared for the 4th Ablation Workshop (1-3 March 2011, Albuquerque, New Mexico).

[2] Lachaud, J., Magin, T., Cozmuta, I., and Mansour, N. N., "A short review of ablative material response models and simulation tools," *7th Aerothermodynamics Symposium*, edited by E. S. Agency, No. to appear, Brugge, Belgium, May 2011, 8 p.

[3] Kendall, R. M., Bartlett, E. P., Rindal, R. A., and Moyer, C. B., "An Analysis of the coupled chemically reacting boundary layer and charring ablator: Part I," *NASA CR*, Vol. 1060, 1968, 96 p.

[4] Thermal Performance Database Team, "Overview of Inter-calibration Results," Oral presentation, 4th Ablation Workshop,1-3 March 2011, Albuquerque, New Mexico.

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[6] Amar, A. J., Calvert, N. D., and Kirk, B. S., "Development and Verification of the Charring Ablating Thermal Protection Implicit System Solver," AIAA paper 2011-144, 2011.

[7] de Muelenaere, J., Lachaud, J., Mansour, N. N., and Magin, T. E., "Stagnation line approximation for ablation thermochemistry," AIAA Paper 2011-3616, 2011.

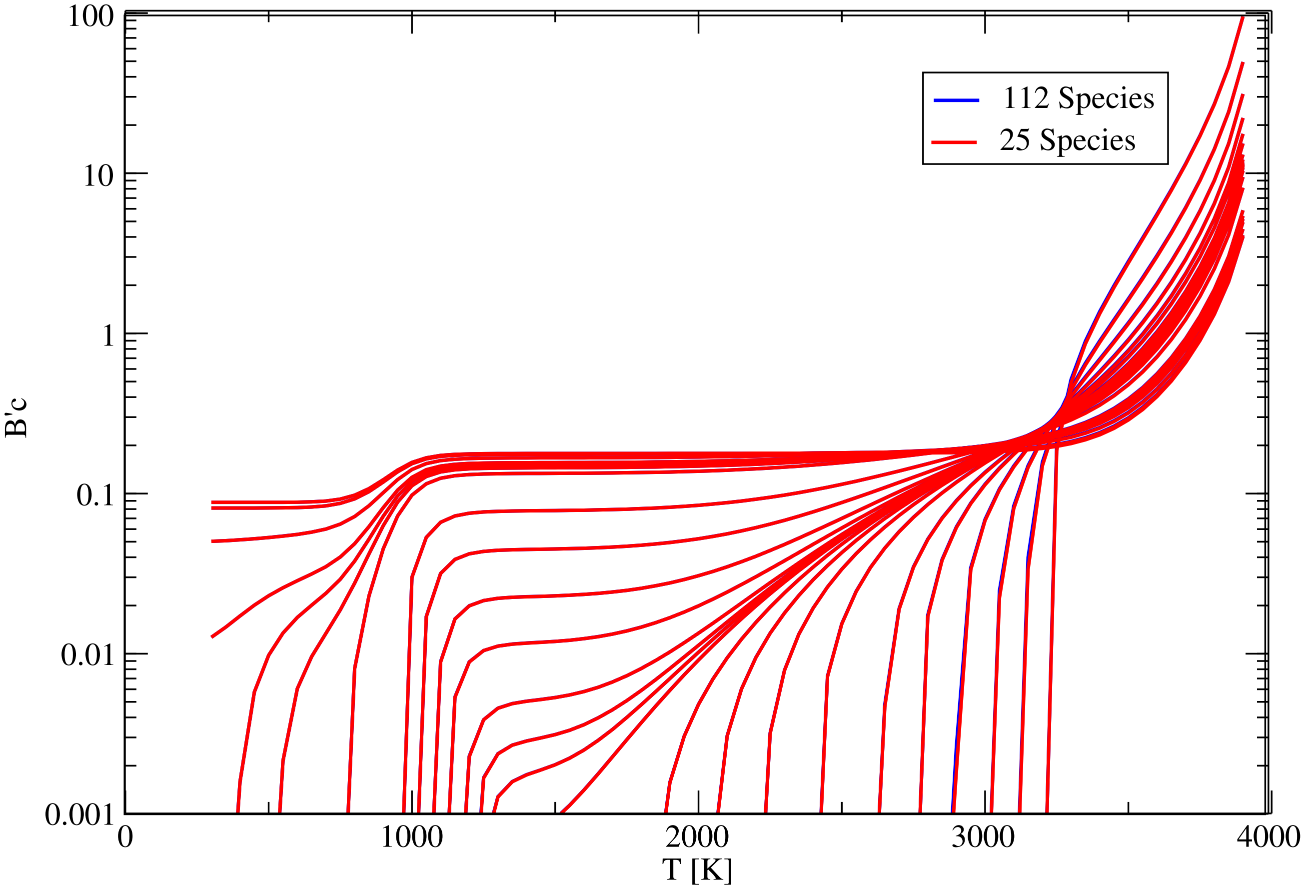
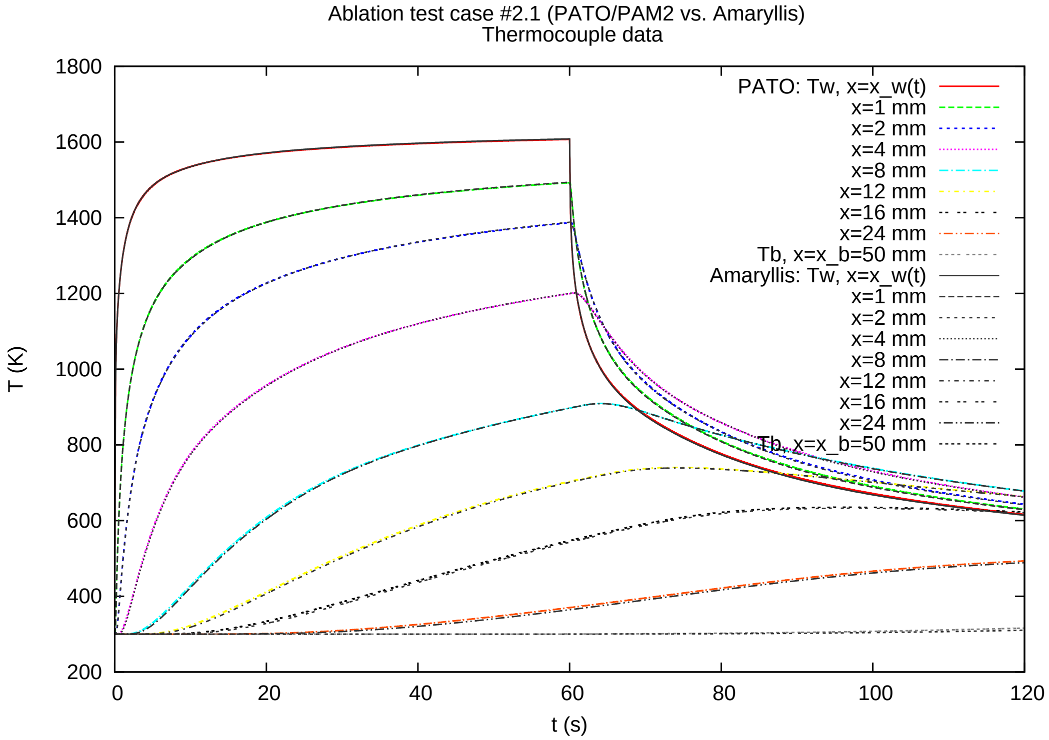
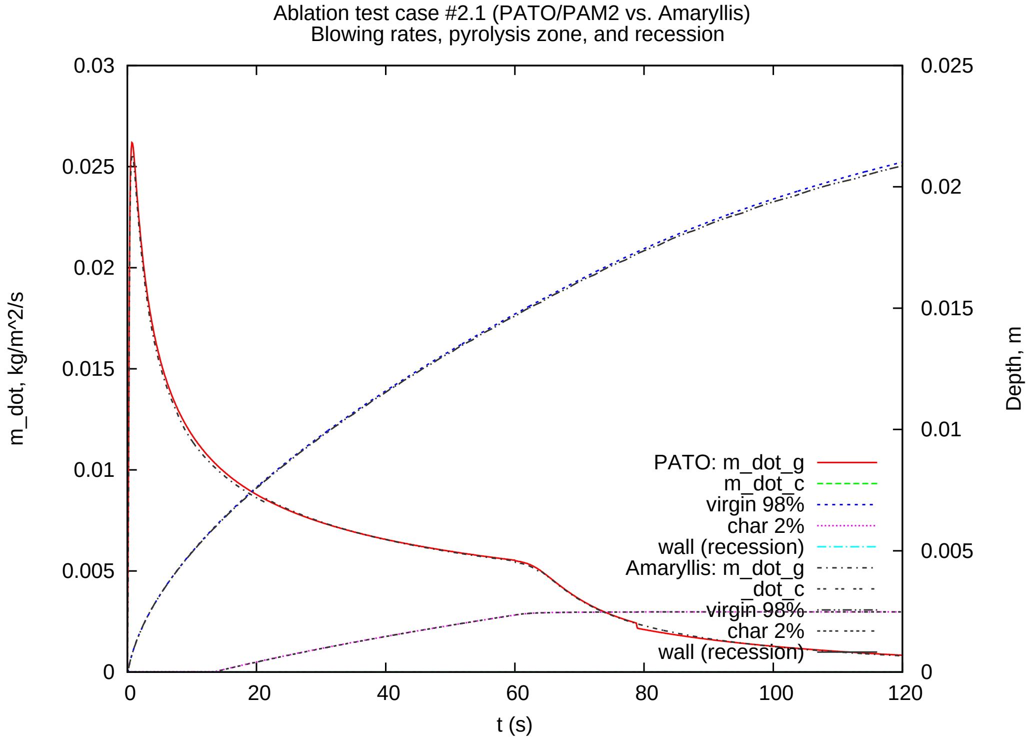
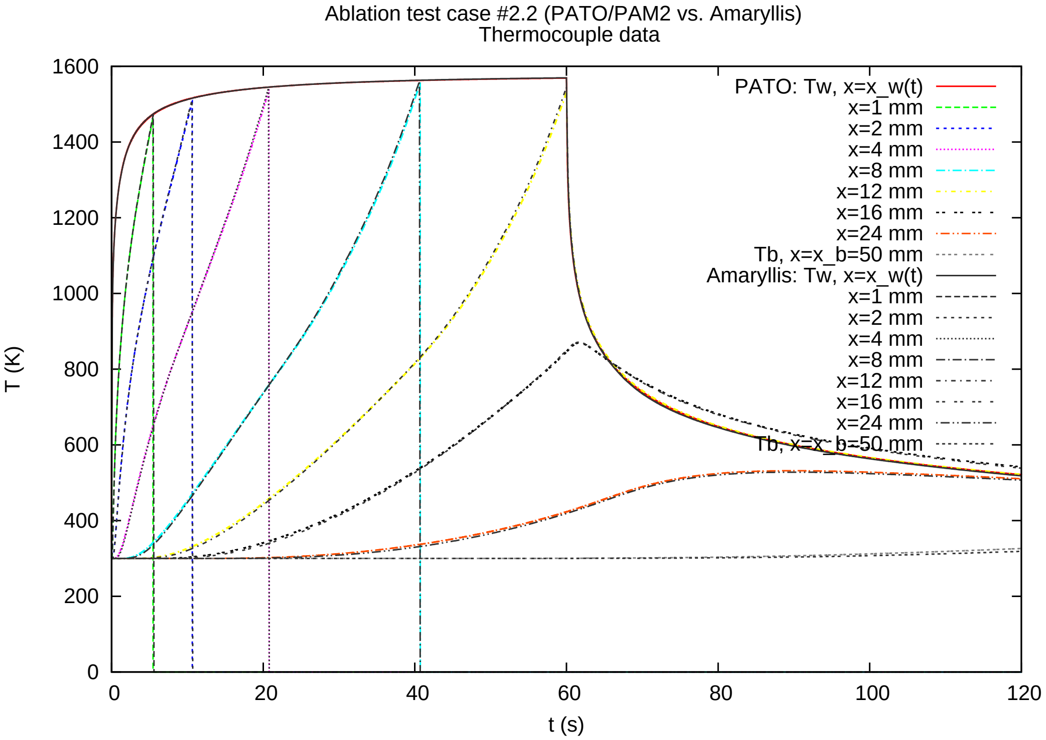
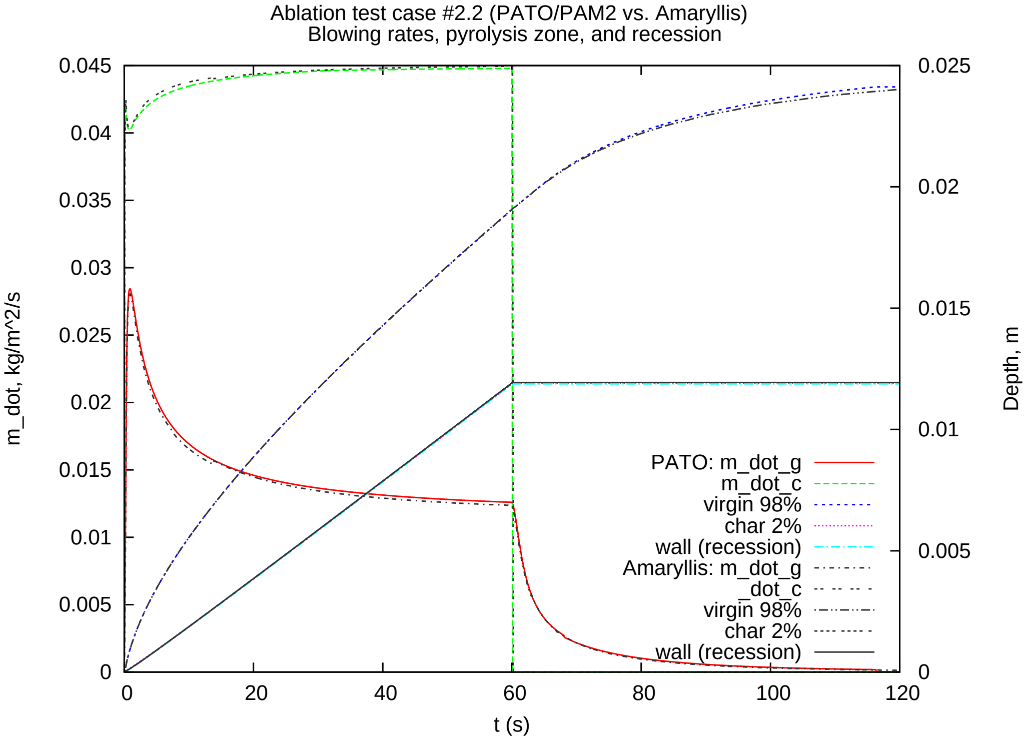


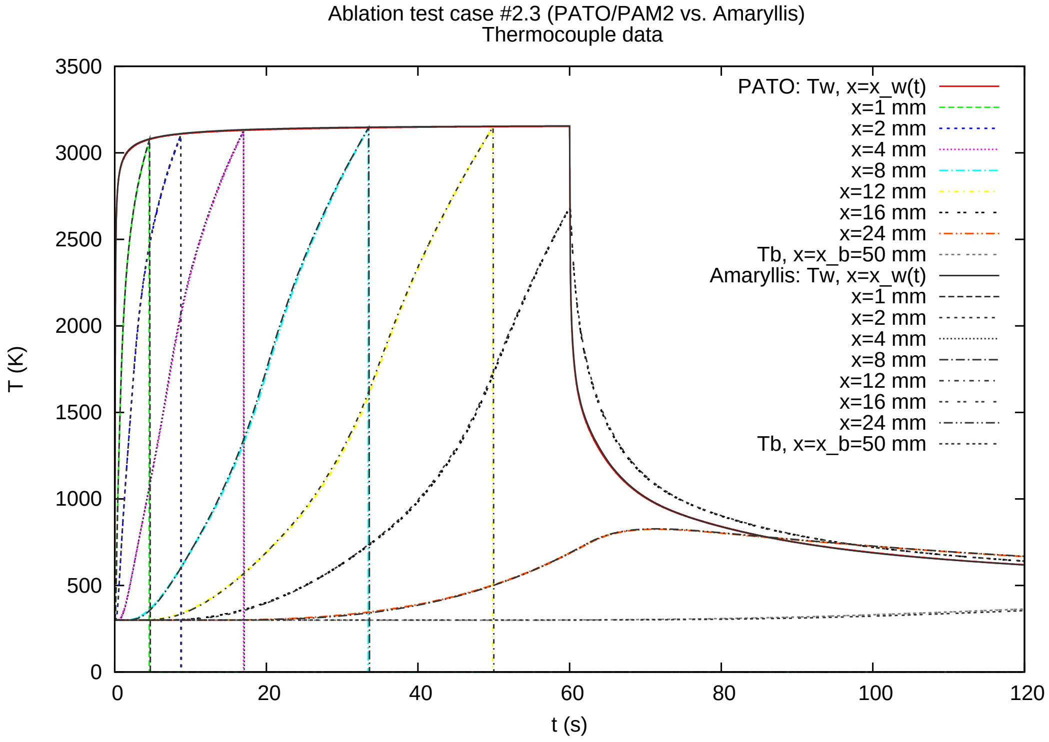
Figure 2: B’ table comparison for the 25-species mixture suggested and a 112-species mixture using the CEA database [Computed with Mutation-B’ by J. de Muelenaere [7]]. The 25-species B’ table is provided in the TACOT_2.2.xls spreadsheet.

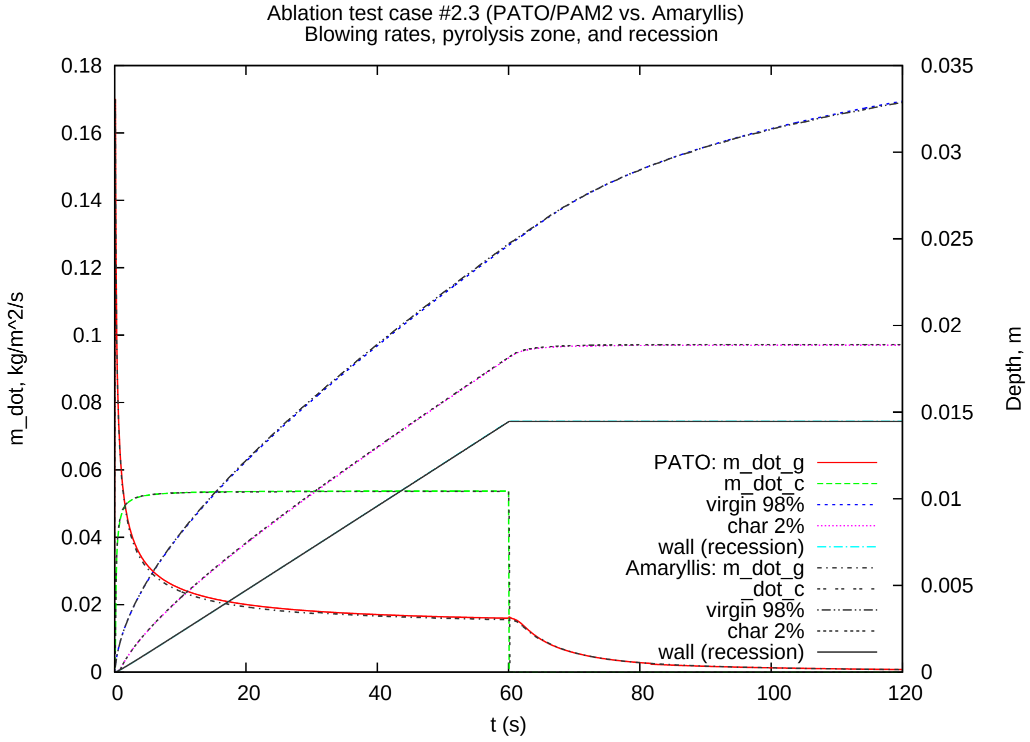

Ablation test case #2.1 (PATO/PAM2 vs. Amaryllis)
Thermocouple data
T (K)
t (s)
1800
1600
1400
1200
1000
800
600
400
200
0
20
40
60
80
100
120
PATO: Tw, x=x_w(t)
x=1 mm
x=2 mm
x=4 mm
x=8 mm
x=12 mm
x=16 mm
x=24 mm
Tb, x=x_b=50 mm
Amaryllis: Tw, x=x_w(t)
x=1 mm
x=2 mm
x=4 mm
x=8 mm
x=12 mm
x=16 mm
x=24 mm
Tb, x=x_b=50 mm


Ablation test case #2.1 (PATO/PAM2 vs. Amaryllis)
Blowing rates, pyrolysis zone, and recession
m_dot, kg/m^2/s
Depth, m
t (s)
0.03
0.025
0.02
0.015
0.01
0.005
0
0.025
0.02
0.015
0.01
0.005
0
0
20
40
60
80
100
120
PATO: m_dot_g
m_dot_c
virgin 98%
char 2%
wall (recession)
Amaryllis: m_dot_g
_dot_c
virgin 98%
char 2%
wall (recession)


Ablation test case #2.2 (PATO/PAM2 vs. Amaryllis)
Thermocouple data
T (K)
t (s)
0
200
400
600
800
1000
1200
1400
1600
0
20
40
60
80
100
120
PATO: Tw, x=x_w(t)
x=1 mm
x=2 mm
x=4 mm
x=8 mm
x=12 mm
x=16 mm
x=24 mm
Tb, x=x_b=50 mm
Amaryllis: Tw, x=x_w(t)
x=1 mm
x=2 mm
x=4 mm
x=8 mm
x=12 mm
x=16 mm
x=24 mm
Tb, x=x_b=50 mm


Ablation test case #2.2 (PATO/PAM2 vs. Amaryllis)
Blowing rates, pyrolysis zone, and recession
m_dot, kg/m^2/s
Depth, m
t (s)
0
0.005
0.01
0.015
0.02
0.025
0.03
0.035
0.04
0.045
0
0.005
0.01
0.015
0.02
0.025
0
20
40
60
80
100
120
PATO: m_dot_g
m_dot_c
virgin 98%
char 2%
wall (recession)
Amaryllis: m_dot_g
_dot_c
virgin 98%
char 2%
wall (recession)


Ablation test case #2.3 (PATO/PAM2 vs. Amaryllis)
Thermocouple data
T (K)
t (s)
0
500
1000
1500
2000
2500
3000
3500
0
20
40
60
80
100
120
PATO: Tw, x=x_w(t)
x=1 mm
x=2 mm
x=4 mm
x=8 mm
x=12 mm
x=16 mm
x=24 mm
Tb, x=x_b=50 mm
Amaryllis: Tw, x=x_w(t)
x=1 mm
x=2 mm
x=4 mm
x=8 mm
x=12 mm
x=16 mm
x=24 mm
Tb, x=x_b=50 mm


Ablation test case #2.3 (PATO/PAM2 vs. Amaryllis)
Blowing rates, pyrolysis zone, and recession
m_dot, kg/m^2/s
Depth, m
t (s)
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0
0.005
0.01
0.015
0.02
0.025
0.03
0.035
0
20
40
60
80
100
120
PATO: m_dot_g
m_dot_c
virgin 98%
char 2%
wall (recession)
Amaryllis: m_dot_g
_dot_c
virgin 98%
char 2%
wall (recession)

18

ABLATION THERMOCHEMISTRY FOR TACOT

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This talk will briefly discuss the ablation thermochemistry data used for the TACOT code comparison test cases. Three areas of interest will be highlighted: codes and numerical methods for solving the thermochemical equilibrium problem, differences in ablation thermochemistry data (Bc and enthalpy) when using the CEA and JANAF databases, and the effect of the choice of pyrolysis gas species will be discussed.

ABLATION TEST-CASE SERIES #3

NUMERICAL SIMULATION OF ABLATIVE-MATERIAL RESPONSE: CODE AND MODEL COMPARISONS

VERSION 1.0, FEBRUARY 16, 2012

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1. INTRODUCTION

The test-case series #3 will be a further extension of the tests defined within the framework of the NASA ablation modelling workshops.[1,2] In order to reduce the amount of work, all tests within test-case series #3, will use the TACOT material defined by Lachaud et al.[2] The main goal of this new series, is to test the 3D modelling capabilities of the participating codes. The first 1D results were presented at the 4th *Ablation workshop*,[3] and together with the results of the second test-case series, will be discussed and analyzed more thoroughly at the 5th *Ablation Workshop, Feb. 28- March 1, 2012, Lexington, Kentucky*.

1.1. Summary of the first test-case

The first test case was defined for the 4th *Ablation Workshop, 1-3 March 2011, Albuquerque, New Mexico*.[1] It was a one-dimensional test case focusing on the in-depth material response - fixed surface temperature and no recession. Three types of material-response codes have been identified:

- Type 1: based on the CMA[4] model or any mathematically equivalent model (heat transfer, pyrolysis, simplified mass transport);
- Type 2: CMA-type + Averaged momentum equation for the transport of the pyrolysis gases;
- Type 3: Higher fidelity codes (chemical/thermal non-equilibrium, etc).

The results had been provided by the participants before the workshop and a summary was presented during the workshop.[3] For type 1 and type 2 codes, differences in the temperature prediction were mostly below 1%.

1.2. Summary of the second test-case series

The definition of the test case series #2 was finalized in Lachaud et al.,[2] and the results of all the participants will be compared at the 5th *Ablation Workshop*. A traditional B' table was provided to facilitate the in-depth material-response comparison but other tables/methods could be used. A specific test-case dedicated to the estimation of the ablation rate was also proposed. A total of four tests were defined:

- 2.1: low heating, no recession (targeted surface temperature of about 1644 K, cf. test-case 1) - non-physical intermediate case without recession in preparation for 2.2.
- 2.2: low heating (same as test case 2.1), recession

- 2.3: high heating, recession (targeted surface temperature of about 3000 K)
- 2.4: computation of the ablation rate of the material of the second test case for a temperature range of 300K-4000K and an air pressure of 101325 Pa (1 atm.). The B'-table format was used to enable visual comparison.

2. DESCRIPTION OF THE THIRD TEST-CASE SERIES

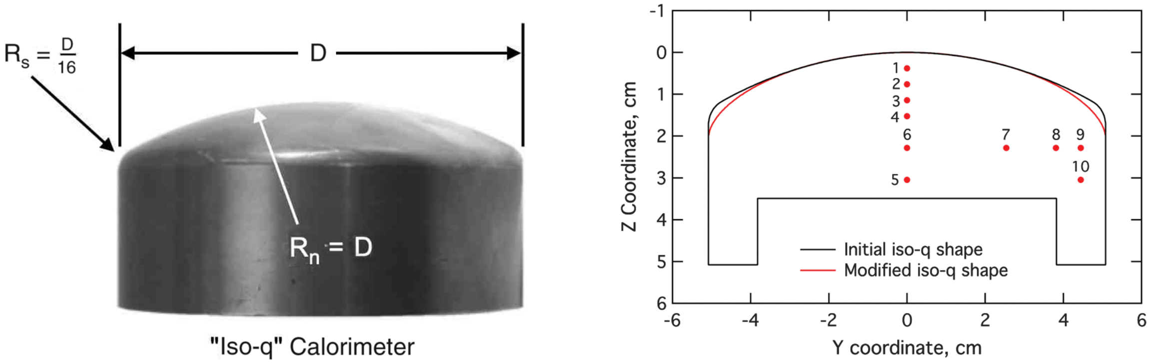
In series #3 two test cases are foreseen, the first test-case is mandatory while the second one will be discussed by the participants. Both tests will be presented at the 5th *Ablation Workshop, Feb. 28- March 1, 2012*, and the tests will be performed by all the participants in the ablation modeling working group (dates discussed during 5th *Ablation Workshop*).

- The mandatory test: This test consists of an "iso-q" calorimeter[5,6] made of TACOT subjected to an enthalpy form heat flux. A total of three tests are performed where every tests has an increasing level of complexity, namely:
  - An axis-symmetric/3D model with an isotropic version of TACOT.
  - The same model but with an orthotropic version of TACOT.
  - A full 3D model with a non-axis-symmetric heat load.
- The optional tests: The SPRITE model,[7] using the TACOT material which is subjected to a re-entry trajectory heat load.

3. THE MANDATORY "ISO-Q" TEST-CASE

3.1. Geometry of the test specimen

The geometry of the mandatory test-case is given in Figure 1, where the diameter D equals 10.16 cm. The "iso-q" test-case is chosen because it was shown[5,6,8] that the ablation will be almost uniform along the surface. As a consequence the shape of the test-specimen will not change during the analysis, and the flow and thermal-structure analysis are decoupled, i.e. the heat load will not change during ablation.



(a) iso-q test specimen

(b) position of the thermo-couples

Figure 1: Definition of the geometry and dimensions of the iso-q test specimen.[5,6,8]

In Figure 1(b) and Table 1 we see the position of the thermo-couples, for which the temperature evolutions have to be post-processed. The thermo-couples are positioned symmetrically with respect to the axis of axis-symmetry (Z-axis). Because both the geometry and the heat load are axis-symmetric, resulting in axis-symmetric results.

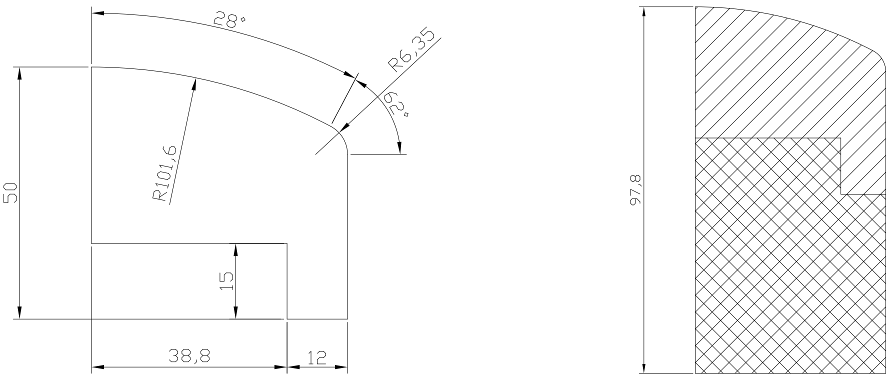
The outer geometry of the specimen is completely defined by the additional assumption that the tangents of the two circles (s,n) (see Figure 1(a)) and the circle (s) and the vertical line, at their intersection points are identical. With these assumptions the dimensions given in Figure 2(a) are obtained, and the following coordinate data can be derived:

- position of the $circle_n$ - $circle_s$ intersection point ($y = 4.679$ cm, $z = 1.174$ cm),

Table 1: Coordinates of the thermo-couples.

TC	Y-coordinate [cm]	Z-coordinate [cm]	TC	Y-coordinate [cm]	Z-coordinate [cm]
1	0.00	0.381	6	0.00	2.286
2	0.00	0.762	7	2.540	2.286
3	0.00	1.143	8	3.810	2.286
4	0.00	1.524	9	4.445	2.286
5	0.00	3.048	10	4.445	3.048

- position of center of rotation of $circle_s$ ($y = 4.445$ cm, $z = 1.736$ cm),
- position of the $circle_s$ - vertical line intersection ($y = 5.080$ cm, $z = 1.736$ cm).



(a) iso-q test specimen (b) iso-q specimen + support structure

Figure 2: The dimensions [mm] of the iso-q specimen + support structure.

Besides the "iso-q" specimen, a support structure is defined in Figure 2(b). Although the support structure will in general be made of a different material, here we will also assume it is also made of TACOT, and that the contact between the "iso-q" specimen and the support structure is perfect. It is therefore allowed to create one continuous mesh/discretization for the "iso-q" and the support structure. With this geometrical data, the participants will be able to construct their numerical (mesh/grid) models.

3.2. Loads and boundary conditions

The test-specimen is subjected to a similar heat load as applied in test 2.3 of test-case series #2. The specimen will be subjected to a convective heating during the first 40 seconds, and it will cool-down for 1 minute under the hypothesis of radiative cooling only. The initial conditions are: $p_0 = 1$ atm (101325 Pa), $T_0 = 300$ K. The initial gas composition in

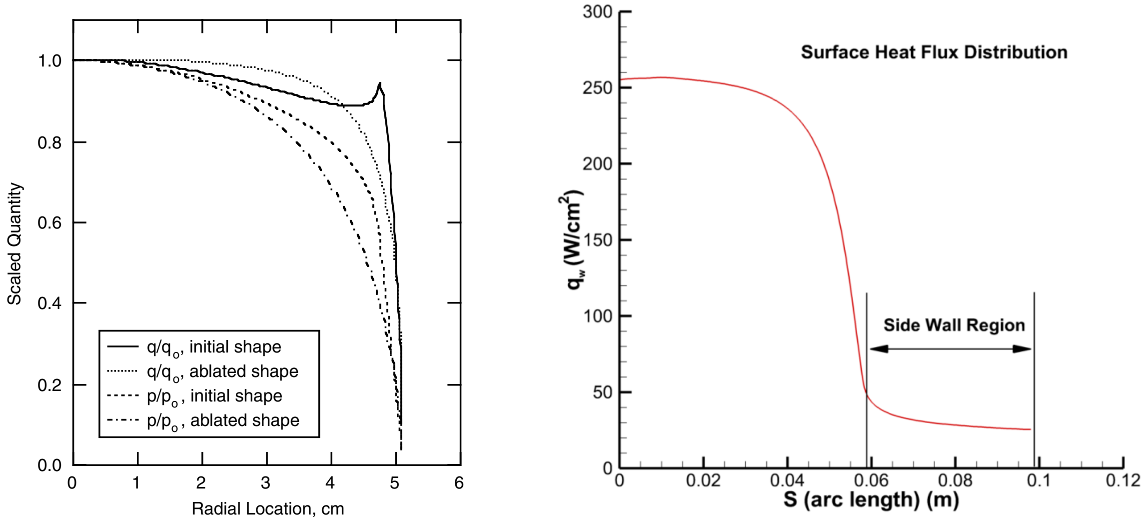
Table 2: Summary of the environment properties. Please use linear interpolation during the 0.1s heating and cooling periods (linear ramping).

time (s)	$\rho_e u_e C_H(0)$ (kg$\cdot$ m$^{-2}\cdot$ s^{-1})	h_e (J$\cdot$ kg^{-1})	p_w (Pa)
0	0	0	101325
0.1	0.3	$2.5 \cdot 10^7$	101325
40	0.3	$2.5 \cdot 10^7$	101325
40.1	0	0	101325
120	0	0	101325

the material is left open. For type 1 and 2 codes, pyrolysis gas in thermal equilibrium is the usual practice. For type 3 codes, it is suggested to start with air. The time-dependent boundary-layer properties are summarized in table 2. The other boundary-layer assumptions/properties are as follows for the code comparison:

- The factor for the blowing-correction correlation used is the CMA model is taken as $\lambda = 0.5$.
- Heat and mass transfer assumptions in the boundary layer: $Pr = Le = 1$
- Re-radiation is active during the entire analysis $[q_r = \varepsilon\sigma(T_w^4 - T_\infty^4)]$. Due to the convex shape of the test-specimens, a view factor of 1 is used. The infinity temperature is chosen to be $T_\infty = 300$ K .
- Use the wall enthalpy (h_w) and the B'_c table provided in the TACOT_2.2.xls file for code comparison.

The above definition of the heat flux ($q(T_w,t)$) is only 1D and applies to the stagnation point only. In order to extend it to the axis-symmetric geometry of Figure 2(b) we will use the heat flux distribution around the "iso-q" calorimeter + support structure, calculated by Dec et.al.[9] and Milos and Chen.[5] In Figure 3(a) the variation of the heat flux and pressure along the test-specimen is given as a fraction of stagnation point load ($q_0, p_0 = p_w$), for the initial and ablated shape. The ablated shape is shown in Figure 1(b), which only has a small local deformation superimposed on an otherwise uniform surface recession.[5] In order to have a uniform recession during the analysis we have to use the q/q_0 values of the ablated shape. Here we will



(a) Heating and pressure distributions[5] for initial and slightly ablated shapes

(b) heating distribution for the iso-q specimen[9]

Figure 3: Heating and pressure distributions[5,9] for the iso-q specimen.

Table 3: Distribution of the $q_w/q_w(0)$ values as a function of the Y- and Z-coordinate (derived from Figure 3(b)).

s (cm)	Y-coord. (cm)	Z-coord. (cm)	$q_w/q_w(0)$	s (cm)	Y-coord. (cm)	Z-coord. (cm)	$q_w/q_w(0)$
0.00	0.000	0.000	1.000	5.50	5.068	1.617	0.476
2.00	1.987	0.196	1.000	5.75	5.080	1.864	0.261
3.00	2.957	0.439	0.971	6.00	5.080	2.114	0.169
3.50	3.431	0.597	0.955	6.50	5.080	2.614	0.137
4.00	3.898	0.777	0.925	8.00	5.080	4.114	0.111
4.50	4.354	0.980	0.863	10.00	5.080	6.114	0.101
5.00	4.800	1.209	0.743	13.70	5.080	9.780	0.101

use the $q_w(s)$ distribution given by Dec at.al.[9] in Figure 3(b), because it is given in more detail. The pressure is held constant both in time and along the outer surface. The pressure distribution calculated in Milos and Chen[5] is valid for an impermeable "iso-q" calorimeter, while TACOT will allow for some equalization of the pressure, which will not be modelled in the series #3 test-cases.

For this test-case we will thus apply the heat-flux and pressure profile defined in Figure 3(b), where we premultiply $\rho_e u_e C_H(0)$ with the $q_w/q_w(0)$ values in Table 3. We will use the TACOT wall enthalpy h_w and ablation rate B'_c values, obtained for a constant pressure $p_w = p_0$ of 101325 Pa. For the back-side of the support structure we assume an adiabatic, and impermeable for gas, boundary condition.

3.3. Axis-symmetric/3D model

Because the model has an axis-symmetric shape, an axis-symmetric discretization will in principle suffice. Depending on the availability of different numerical models (in the participating codes) the participants may decide to use a 3D segment model instead of an axis-symmetric model. Both the 3D segment model and the axis-symmetric model will give the same results, and can be used for both the isotropic and orthotropic material model.

3.3.1. Model with an isotropic material

The TACOT material definition (TACOT_2.2.xls) is an isotropic definition, and can thus be applied directly to the axis-symmetric/3D model.

3.3.2. Model with an orthotropic material

One of the goals of this test-series, is to compare the modelling capabilities of the different codes. One of the modelling capabilities, of practical interest, is to model orthotropic materials. For example PICA[5] is known to be orthotropic, where the Through The Thickness conductivity is lower that the isotropic conductivity, and the In Plane conductivity is higher than the isotropic conductivity. We therefore propose to use an orthotropic model, where the conductivities are defined via multiplication factors ($\alpha_1 = 0.9, \alpha_2 = 1.1$) for the isotropic conductivity of the TACOT model.

$$\begin{vmatrix} \lambda_{TTT} & 0 \\ 0 & \lambda_{IP} \end{vmatrix} = \begin{vmatrix} \alpha_1 & 0 \\ 0 & \alpha_2 \end{vmatrix} \lambda_{\text{isotropic}} \tag{1}$$

The through the thickness direction is aligned with the axis of axis-symmetry (Z-axis in Figure 1).

3.4. A full 3D model with a 3D heat load definition

A final functionality that will be tested within series #3, is the full 3D modelling capabilities of the participating codes. Because finding a fully 3D physical test is not obvious, we have decided to perform a non-physical test, which is similar in concept to the test shown in Lachaud and Mansour.[10] Here we will use a full 3D "iso-q" model with the orthotropic TACOT material defined in section 3.3.2.

While the pressure distribution will not be modified, the heat-load distribution (from section 3.2) will be modified in such a way that it becomes non-symmetric. The q/q_0 distribution will be multiplied, with a Gaussian distribution, in such a way that a localized heat-flux peak will be added on top of the existing distribution. The multiplication factor will be:

$$f(x,y) = 1 + \beta e^{-\frac{1}{2\sigma^2}\left[(\mu_x - x)^2 + (\mu_y - y)^2\right]} \tag{2}$$

The Gaussian is determined by the position of its average values ($\mu_x = 0.0$ cm, $\mu_y = 1.0$ cm) and the radius ($2\sigma = 1.0$ cm) in which 95.4 % of the additional power is applied. The nominal heat flux q/q_0 will be increased by a multiplication value of β (= 0.3). This multiplication function will result in a 3D localized heat flux, and thus a 3D solution.

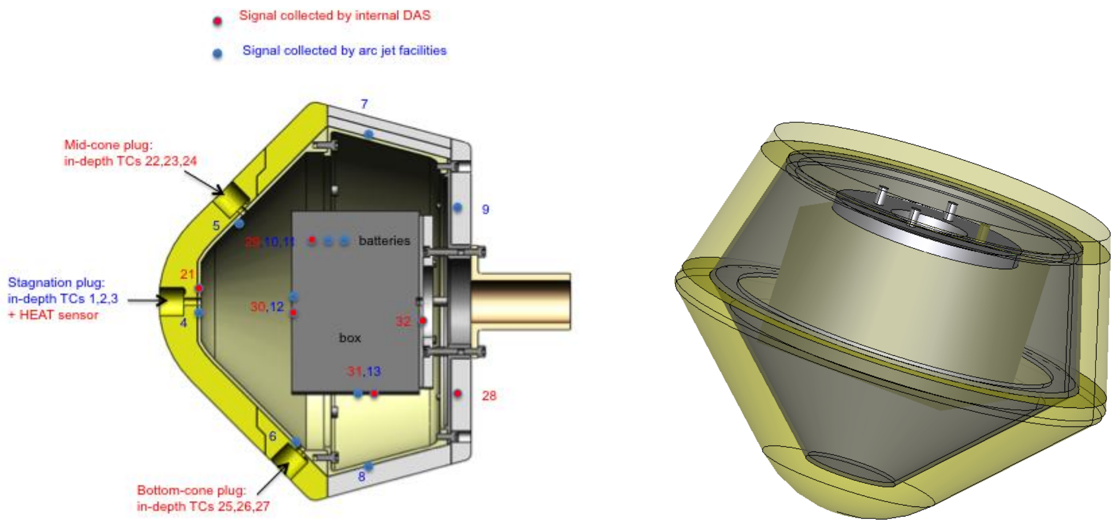
4. THE SMALL RE-ENTRY PROBE TEST-CASE

After testing the participating codes, on all the necessary functionalities for an industrial type application, a re-entry probe model is a logical next step. As an example the SPRITE model, described by Empey et al.,[7] is used. The definition of the small re-entry probe test case is not yet finalized, and will be the subject of discussions between the workshop participants. The questions that need to be answered are:

- Will we apply a realistic re-entry load, and if so who will be capable and willing to supply this?
- Do we need to model radiative heat exchange (between structure and instruments) inside the capsule?
- How will the geometry of the test-case be defined:
  - will a description, like in Figure 2, be given?
  - will a full 3D CAD model be supplied?
  - will a finite element mesh be supplied?
- what are the results we would like to obtain?
- Which of the participants is able and willing to do this test?

4.1. Geometry of the test specimen

In Figure 4(a) we see a cross section of the SPRITE model given in the paper of Empey et al.[7] From this paper a 3D model of the probe has been re-created, and it is given in Figure 4(b). The model shown, is available as a CAD file (STEP format) and can be obtained from the authors.



(a) Cross-section and instrumentation (b) Re-created CAD model

Figure 4: Definition of the SPRITE probe.[7]

4.2. Material definition

For the SPRITE model we will again use the orthotropic version of the TACOT material, as defined in section 3.3.2. In this case the IP direction is perpendicular to the axis of axis-symmetry, i.e. the TTT direction is only perpendicular to the outer surface at the stagnation point.

4.3. Loads and boundary conditions

A uniform initial temperature of 300 K is assumed, after which a re-entry heat flux is applied. This heat flux (convection, radiation) will depend on wall temperature, time and varies with location over the heat shield. The definition of this heat flux will be discussed between the participants.

5. MATERIAL DATA

The material properties for this test-case series are provided and explained in the spreadsheet TACOT_2.2.xls. Recent updates:

- B' table updated (July 28, 2011)
- Equilibrium properties of the pyrolysis gases up to 4000K (June 2011)

6. CODE OUTPUT AND COMPARISON OF THE RESULTS

The code output described in this section will only apply to the results of section 3. The output for the re-entry vehicle will depend on it's definition, which is the subject of ongoing discussions. The results will be supplied in ASCII file format, which contain the following results (with an output frequency of $0.1\,s$):

- The temperature at the position of the stagnation point and of the 10 thermo-couples will be post-processed. The position of the thermo-couples are defined in Table 1 and Figure 1.
- For the same points (stagnation point and the thermo-couples) also the density will be post-processed.
- The blowing rates, the surface recession and the pyrolysis zone thickness, will be post-processed at the stagnation point. The mass and the position of the centre of gravity, of the "iso-q" specimen, will be calculated.The values to post-process are:
  - Blowing rates: The blowing rates $\dot{m}^g$ and $\dot{m}^c$ are calculated at the outer surface.
  - Pyrolysis zone thickness: The thresholds, to calculate the location of the pyrolysis and char fronts, are defined as: $\rho_v(98\%) = \rho_c + 0.98(\rho_v - \rho_c)$; $\rho_c(2\%) = \rho_c + 0.02(\rho_v - \rho_c)$. The distance is calculated w.r.t. the initial outer surface.
  - Surface recession: The displacement of the point w.r.t. the original position is calculated.
  - Mass: The total mass of the "iso-q" specimen will be calculated as a function of time.
  - Y-coordinate: The y-coordinate of the centre of gravity, of the "iso-q" specimen, as a function of time.

Output format desired:

time (s)	Tw (K)	T1 (K)	T2 (K)	T3 (K)	...	T8 (K)	T9 (K)	T10 (K)
0	3.000e2	3.000e2	3.000e2	3.000e2	3.000e2	3.000e2	3.000e2	3.000e2
0.1	9.651e2	3.225e2	3.000e2	3.000e2	3.000e2	3.000e2	3.000e2	3.000e2
0.2	1.076e3	3.956e2	3.039e2	3.000e2	3.000e2	3.000e2	3.000e2	3.000e2
etc.	...	...	...	...	...	...	...	...

Table 4: Output format for the temperature file: CodeName_Energy_TestCase_3-i.txt

time (s)	rhow (kg/m3)	rho1 (kg/m3)	rho2 (kg/m3)	...	rho10 (kg/m3)
0	2.800e2	2.800e2	2.800e2	2.800e2	2.800e2
0.1	2.7900e2	2.800e2	2.800e2	2.800e2	2.800e2
0.2	2.7500e2	2.800e2	2.800e2	2.800e2	2.800e2
etc.	...	...	...	...	...

Table 5: Output format for the density file: CodeName_Density_TestCase_3-i.txt

Result files need to be generated for the three test cases of section 3, and the i in the file names will refer to:

- $i = 1$: Model with an isotropic material,
- $i = 2$: Model with an orthotropic material,
- $i = 3$: A full 3D model with a 3D heat load definition.

time (s)	m_dot_g (kg/m2/s)	m_dot_c (kg/m2/s)	Virgin 98%	Char 2%	recession (m)	Mass (kg)	Y-coord. (m)
0	0	0	0	0	0	1.200E-02	1.200E-02
0.1	5.063e-3	0	0	0	0	1.200E-02	1.200E-02
0.2	1.340e-2	0	1.781e-4	2.130e-5	0	1.200E-02	1.200E-02
etc.	...	...	...	...	...	...	...

Table 6: Output format for the pyrolysis and ablation-response file: CodeName_Mass_TestCase_3-i.txt

7. PRELIMINARY RESULTS

The results shown are generated with SAMCEF Amaryllis, and serve as a baseline for visual comparison for the test cases. Please do not give them more credit than they deserve and use them for sanity check rather than for comparison.

8. ACKNOWLEDGMENTS

We would like to thank you in advance for any comment that will help to improve the clarity of this document. Please send your comments to the authors.

9. REFERENCES

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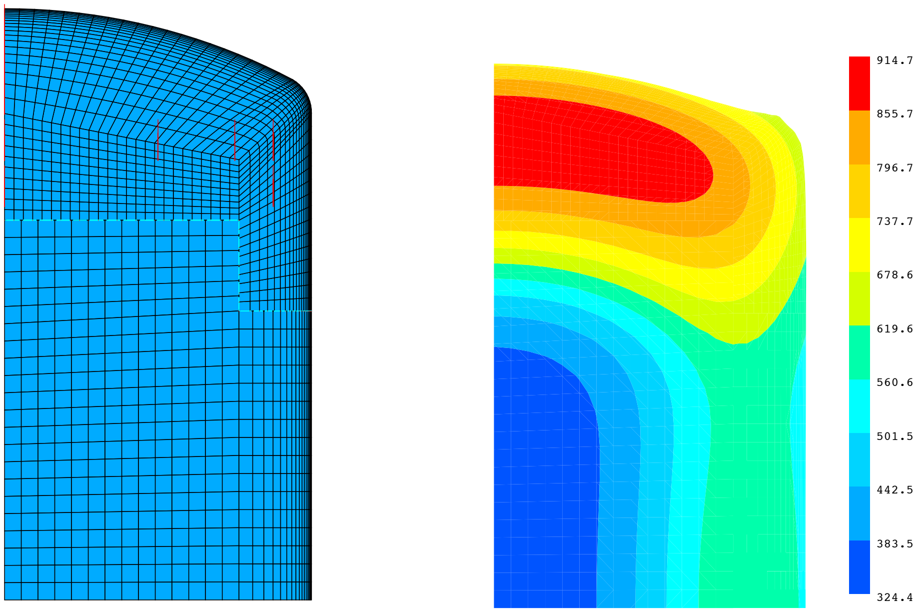
Initial results of test-case 3.1



(a) axis-symmetric mesh distribution

(b) Temperature distribution on deformed mesh at t = 120 seconds

Figure 5: Test3.1: Mesh and temperature distribution of the test-specimen plus the support structure.

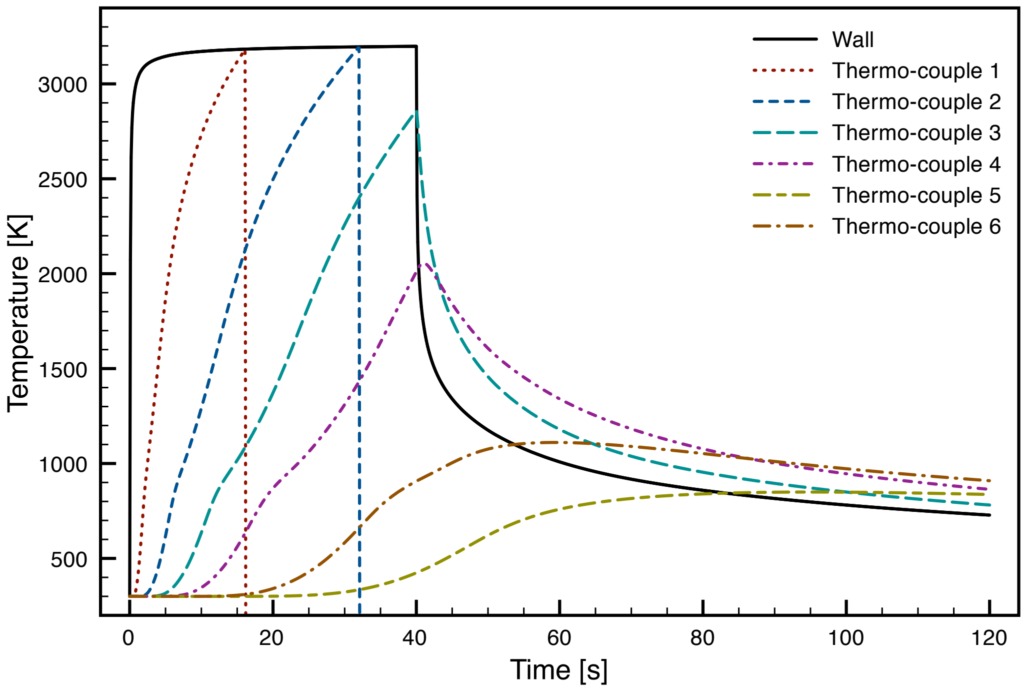


Figure 6: Test3.1: Temperature evolution of the wall and the thermo-couples 1 till 6.

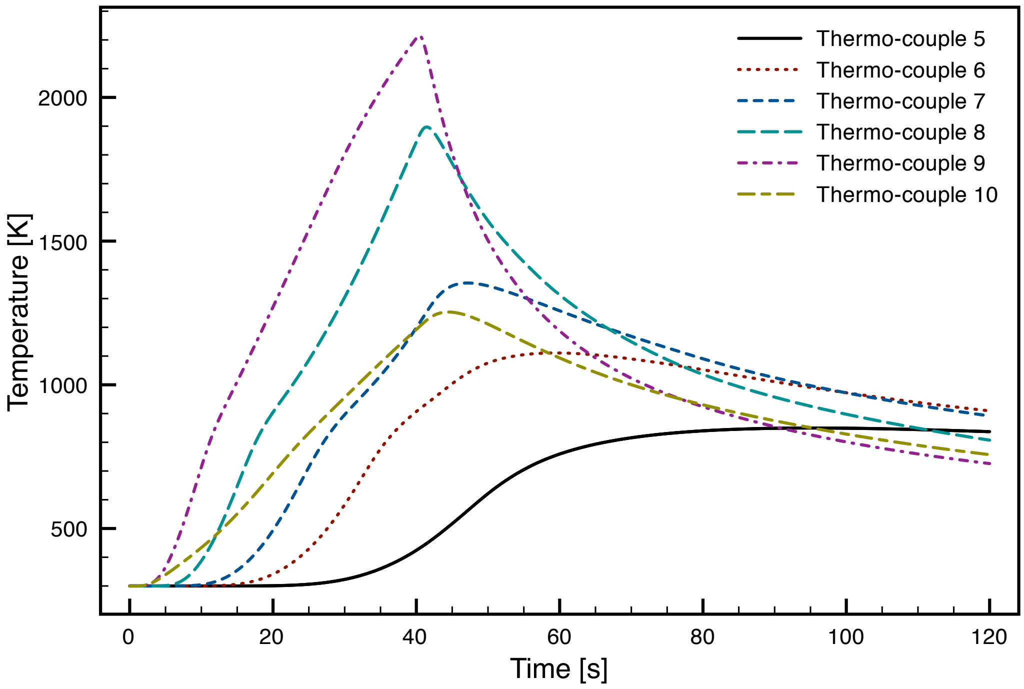


Figure 7: Test3.1: Temperature evolution of the thermo-couples 6 till 10.

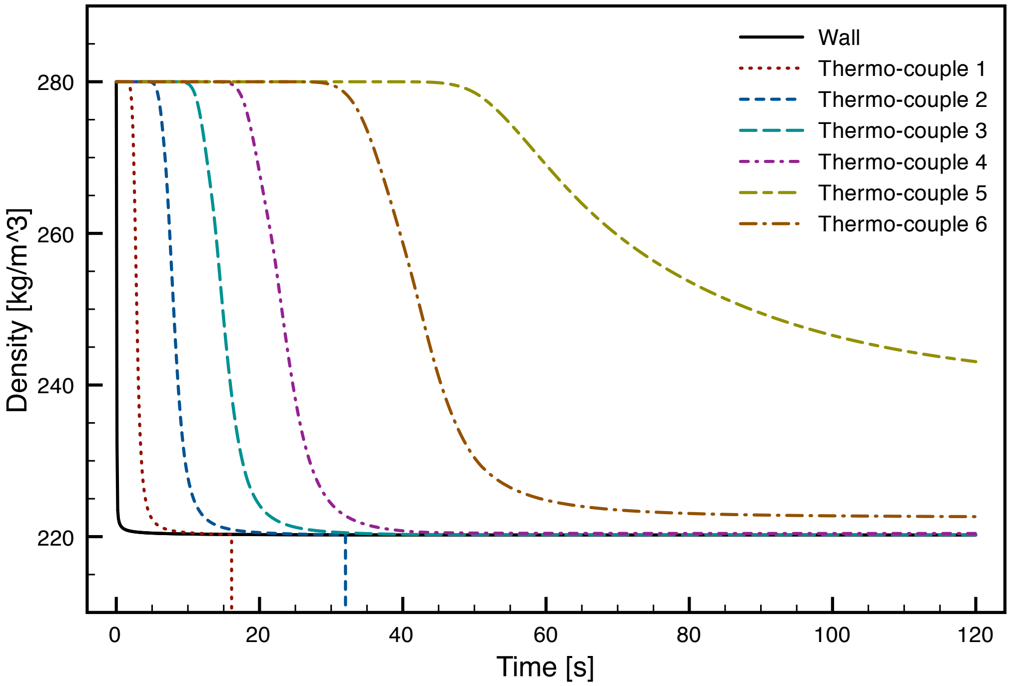


Figure 8: Test3.1: Density evolution of the wall and the thermo-couples 1 till 6.

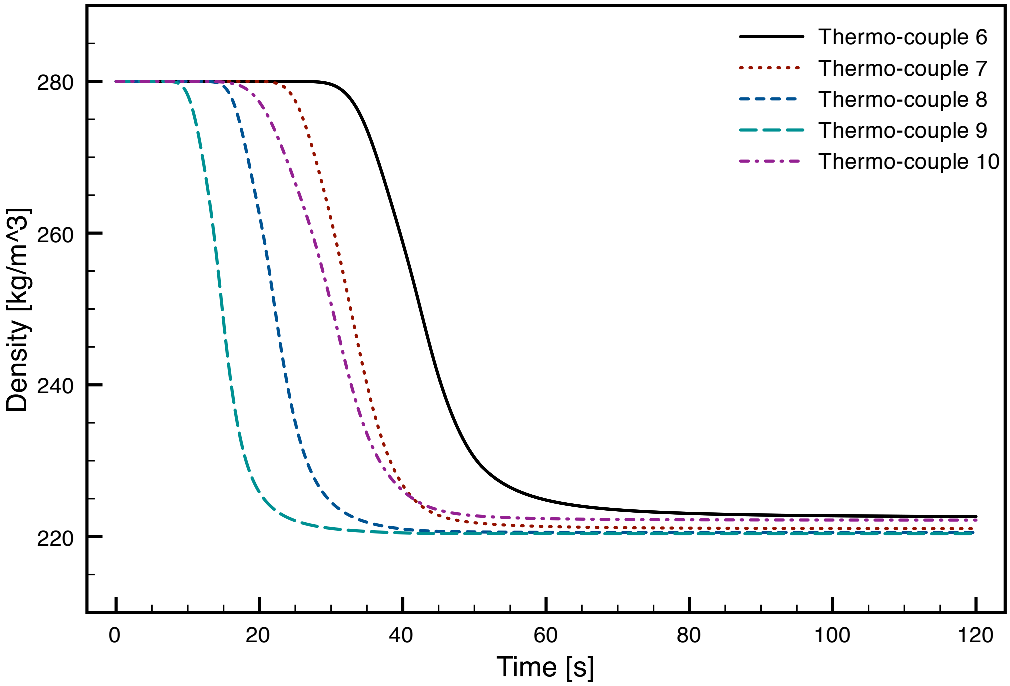


Figure 9: Test3.1: Density evolution of the thermo-couples 6 till 10.

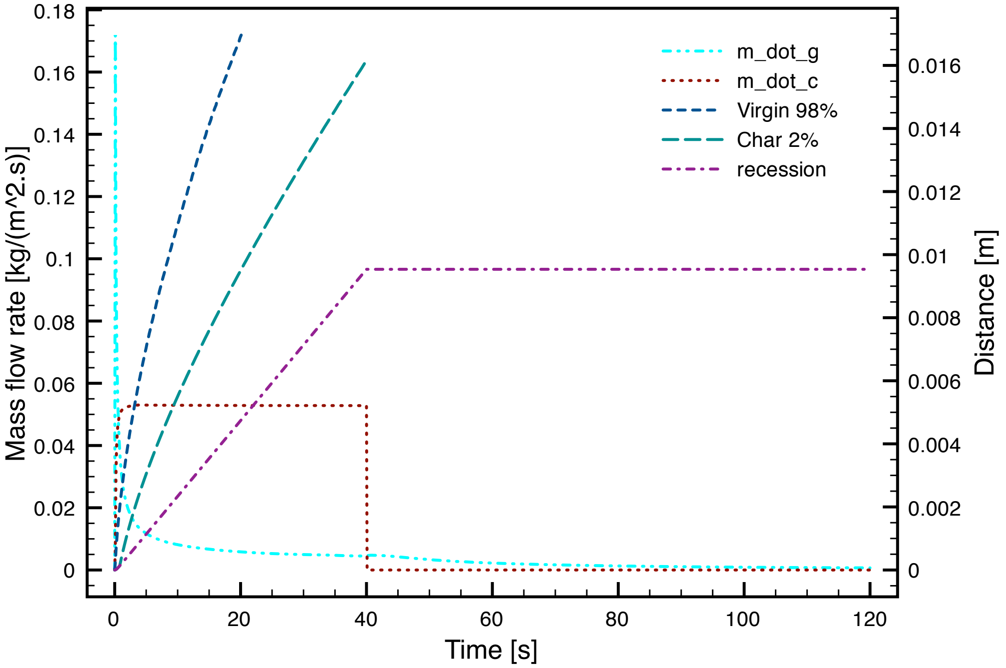


Figure 10: Test3.1: Mass flow rate, wall recession, and (partial) char thickness at the stagnation point.

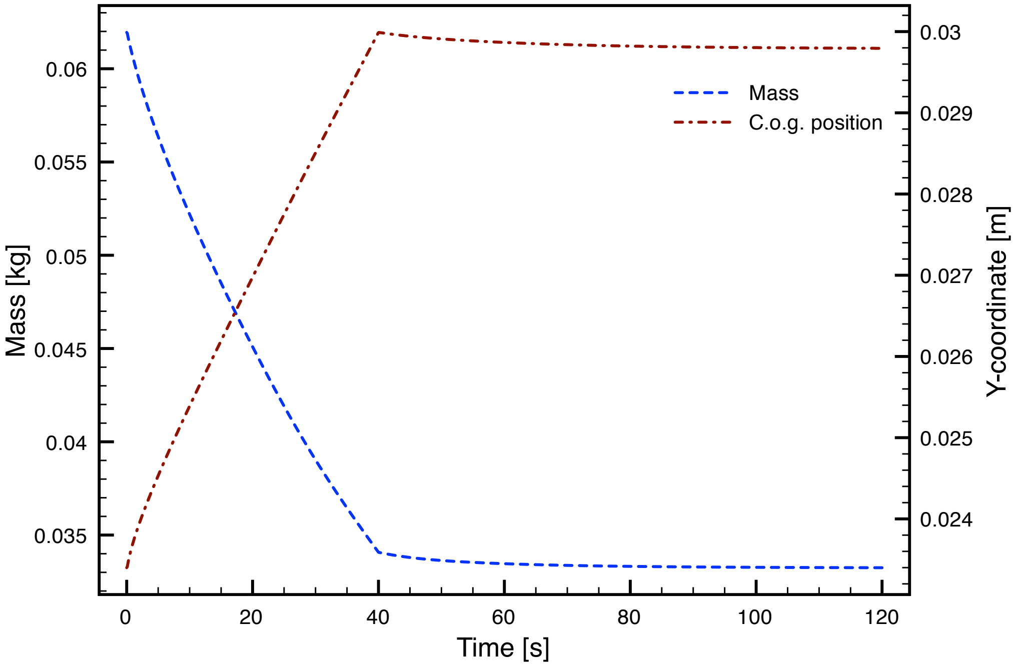


Figure 11: Test3.1: Mass and centre of gravity evolution, of the "iso-q" specimen.

EXPERIMENTAL TEST CASE

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Over the last several years, there has been increasing demand from ablation scientists to have open access to an ablative material. On the modeling side, researchers want to verify and test the various models used in their codes. Similarly, experimentalists want to benchmark their measurement techniques and study specific aspects of the ”real” materials. Unfortunately, most materials used for current re-entry applications fall under ITAR regulations, and are therefore unavailable to international researchers. This has the effect of inhibiting collaboration with academia, even within US institutions. Moreover, even within the confines of the ITAR regulations, data exchange is tedious and time consuming.

It is the hope of this panel to explore and propose solutions to this problem. One possible solution is to study a non-flyable, non-ITAR restricted material that is currently used for commercial applications. That material, if judged suitable for such a task, could be used as a basis for experimental and theoretical ablation studies. Other solutions, such as designing a light weight, non-flyable ablator similar to ablators in current use, will also be explored. Finally, the feasibility of re-regulating restricted materials will also be discussed.

In the event of a material being selected, it is also the hope of this panel to start devising an experimental inter-comparison exercise, which will provide results to calibrate and verify material response codes.

ABLATION MODELING OF A SOLID ROCKET NOZZLE

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MODELING OF HEAT TRANSFER ATTENUATION BY ABLATIVE GASES DURING THE STARDUST RE-ENTRY

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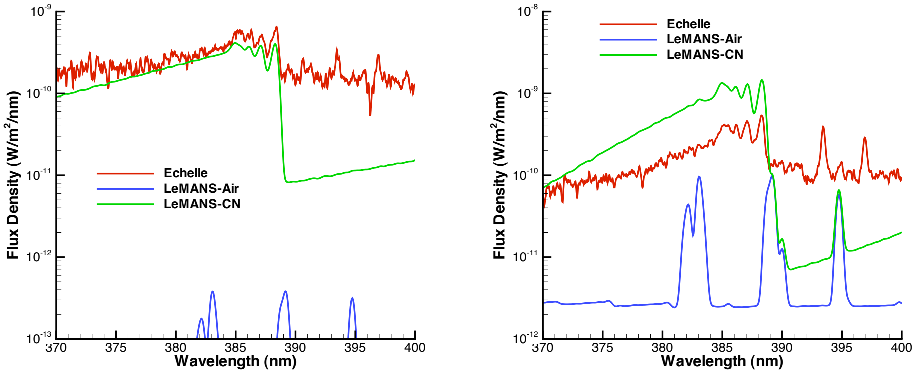
The great majority of modern space vehicles designed for planetary exploration use ablative materials to protect the payload against the high heating environment experienced during re-entry. In order to properly model and predict the aerothermal environment of the vehicle, it is imperative to account for the gases produced by ablation processes. In the case of charring ablators, where an inner resin is pyrolyzed at a relatively low temperature, the composition of the gas expelled into the boundary layer is complex and may lead to thermal chemical reactions that cannot be captured with simple flow chemistry models. In order to obtain better predictions, an appropriate gas flow chemistry model needs to be included in the CFD calculations. The effects of allowing such gaseous species to form in the flow field have notable repercussions on the amount of heat fluxes to the surfaces.

The present study examine the effects of blowing of pyrolysis gas in the outer flow field. Using six points on the Stardust entry trajectory at the beginning of the continuum regime, from 81 km to 69 km, the various components of the heat flux are compared to air-only solutions. Although an additional component of the heat flux is introduced by mass diffusion, this additional term is mainly balanced by the fact that the translational- rotational component of the heat flux, the main contributor, is greatly reduced. Although a displacement of the shock is observed, it is believed that the most prominent effects are caused by a modification of the chemical composition of the boundary layer, which reduces the gas phase thermal conductivity.

In order to validate the models, a flow field solution is used to perform analysis of the CN radiative spectral emission using NEQAIR. The result are compared to the experimental data obtained by the Echelle instrument at the 81 km and 71 km trajectory points. The computed results, shown on Fig. 1, are very close to the observed values, which provides increased confidence in the carbon-phenolic-in-air chemistry model, and the overall approach.



(a) 81 km: 34s into re-entry

(b) 71 km: 44s into re-entry

Figure 1: Spectral emission for the Startdust re-entry vehicle at 81 km and 71 km

A RADIATIVE TRANSFER EQUATION SOLVER MODULE FOR COUPLED SIMULATION OF HYPERSONIC FLOW WITH ABLATION

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Accurate numerical modeling of the aerothermal environment around an ablation-cooled hypersonic re-entry vehicle requires high-fidelity models for processes such as non-equilibrium surface themochemistry, non-equilibrium pyrolysis chemistry, multi-scale radiation, spallation and charring. It is expected that, these models when utilized in a coupled manner will be able to accurately capture the possible nonlinear interactions between various phenomena in a computationally efficient manner. Development of a coupled radiative solver is currently being carried out as part of a joint effort between CFDRC, University of Michigan and University of Kentucky to develop a fully coupled method of simulating atmospheric entry flows and response of the thermal protection system. A key aspect of the project is development of a modular radiative transfer equation (RTE) solver which can be used in a tightly coupled manner with any hypersonic flow code. The code will be coupled with latest spectral property databases allowing almost line-by-line accuracy for radiative heat-fluxes on the spacecraft surface while still utilizing a multidimensional RTE formulation. The presentation will focus on architecture of the RTE solver, radiative property models that can be used in the solver and its interfacing with LeMANS aerothermal code for a simple demonstration case. The infrastructure to couple the solver with other codes of interest will be outlined.

CFD ABLATION PREDICTIONS WITH COUPLED GSI MODELING FOR CHARRING AND NON-CHARRING MATERIALS

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To this day, a major objective of TPS design is to reduce empiricism, and to increase fundamental modeling capability through increased understanding. One of the most challenging aspect is the proper coupling between the material response and the external flow field. With this regard, the goal of this research activity is the improvement of the numerical modeling capabilities through the development of advanced CFD tools integrated with Gas-Surface Interaction (GSI) modeling.

Numerical prediction of ablation is ambitious and cpu-time demanding due to the complex multiphase physical and chemical processes that occur. With improvements in computational algorithms and advances in computer hardware, Navier-Stokes based approaches have become the norm in recent years for coupling to material thermal response predictions. The present state of the art in fluid-material coupling is represented by loose coupling of a high-fidelity CFD flow solver with a material thermal response code. In that respect, some major restrictions are still present in these state of the art coupled solutions:

- surface chemical equilibrium assumption
- non-ablating flow field prediction
- simplified diffusion modeling based on transfer coefficient

Chemical equilibrium is a special condition of the general chemical nonequilibrium condition and surface recession rate predicted by the chemical equilibrium surface chemistry is usually reasonably conservative and is considered to be a best alternative when the nonequilibrium computation is too expensive or unlikely to be achieved. The ablation models are currently largely based on the surface equilibrium assumption and the effects and importance of non-equilibrium ablation models coupled with CFD tools are only beginning to be explored. Moreover, the coupling between CFD solver and material response code is often made considering non-ablating flow field solutions assuming a fully/super-catalytic, radiative equilibrium wall. This means that the effect on the flow field solution of the ablation and pyrolysis gas injection and of variable surface temperature are treated only approximately relying on the use of mass and energy transfer coefficients and semi-empirical blowing correction equations. Finally, the ablation rate is generally computed by the material response code using thermochemical tables and extremely simplified diffusion models based on transfer coefficients and semi-empirical relations relating mass and energy transfer.

The objective of this research activity is to remove these major limiting assumptions developing suitable finite-rate GSI models and integrating CFD technology with Computational Surface Thermochemistry (CST) to take into account the effect of surface ablation and pyrolysis gas injection on the flow field and to allow surface ablation and surface temperature distributions to be determined as part of the CFD solution. Because the entire flow field is to be solved with ablative boundary conditions, the film-transfer theory assumption is no longer needed; this will permit to avoid all of the classical approximations such as transfer coefficients, equilibrium thermochemical tables, and blowing correction equations which needs to be used when ablative boundary conditions are not accounted for in the CFD solution. The ablative boundary conditions, based on finite-rate chemistry, species mass conservation and surface energy balance, is discretized and integrated with the CFD code to predict aerothermal heating, surface temperature, gas-phase surface composition, and surface ablation rate. The concentrations of chemical species at wall are determined from finite-rate gas-surface chemical reactions balanced by mass transfer rate. The surface temperature is determined from the surface energy balance assuming steady-state ablation or coupling with a thermal response code. The surface recession rate and the surface temperature are thus obtained as part of the flow field solution. The computational tool developed in this work is used to simulate two sets of experimental data for nozzle material ablation: sub-scale motor tests carried out for the Space Shuttle Reusable Solid Rocket Motor and the static firing tests of the second and third stage solid rocket motors of the European VEGA launcher which use carbon-carbon for the throat insert and carbon-phenolic for the region downstream of the throat.

UNCERTAINTY ANALYSIS OF REACTION RATES IN A FINITE RATE GAS SURFACE MODEL

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A finite–rate–catalytic wall boundary condition incorporated into hypersonic flow simulations is investigated. Benchmark simulations of hypersonic flow over a cylinder are presented using the finite–rate–catalytic model parameterized with a test air–silica chemical model comprising the gas–surface reaction mechanisms and their associated rates. It is demonstrated that backwards recombination rates should not be arbitrarily set but must be consistent with the gas–phase thermodynamics, otherwise a drift from the equilibrium state may occur. The heat flux predicted by the finite rate model lies between non–catalytic and super–catalytic limits depending on the surface temperature. It is found that even for a constant surface temperature, the oxygen recombination efficiencies determined by the model are not only a function of temperature, but also a function of the surface coverage, where recombination efficiencies are seen to rise as coverage decreases. Monte Carlo uncertainty analysis is performed to correlate the influence of individual mechanisms to the stagnation point heat flux and the expected progression of dominant mechanisms is found as the surface temperature is raised. Additionally, it is found that increased surface reactivity increases the chemical heat flux while also altering the boundary layer in a manner that decreases the conductive heat flux. Finally, efforts to use computational chemistry to reduce the uncertainty in individual rates of dominant oxidation mechanisms for oxygen–carbon interactions will be summarized.

COUPLED COMPUTATION OF FLUID AND MATERIAL RESPONSE FOR NON-CHARRING ABLATIVE MATERIALS IN HYPERSONIC FLOW

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Hypersonic vehicles are subjected to high heat loads throughout their flight trajectories, and as a result, some form of thermal protection system (TPS) is required to ensure the vehicle's survival. Accurate prediction of the behavior of these materials in a hypersonic environment is crucial to the efficient design of a hypersonic flight vehicle. It can be very costly and difficult, however, to experimentally replicate the flow conditions found in many hypersonic regimes, and for this reason it is desirable to be able to simulate the behavior of TPS materials under these flight conditions. This study aims to improve the modeling of the coupled fluid-material response problem for TPS materials in realistic hypersonic flows by coupling a hypersonic CFD code with an axisymmetric material response code.

TPS materials can be broadly classified into two main categories: ablative, where there is a mass loss from the material, and non-ablative where there is no mass loss. Ablative materials can be further divided into charring and non-charring materials. Charring ablators undergo internal decomposition of a resin material, which produces a gas that flows out of the material. After the resin has decomposed, a char material is left behind which may begin to recess if the heat load is high enough. Non-charring ablators, on the other hand, lose mass directly from the ablator surface without first undergoing resin decomposition, and so there is some surface recession of the material. The goal of this study is to develop a material response code for non-charring ablative TPS materials that is capable of handling axisymmetric geometries. This material response code is then coupled to LeMANS[1], a hypersonic computational fluid dynamics code, to predict the behavior of non-charring TPS materials in hypersonic flow conditions. This work extends the previously shown coupling of LeMANS with the one-dimensional material response code, MOPAR [2], also developed at the University of Michigan.

The material response code developed in this study uses the Control Volume Finite Element Method [3] (CVFEM), and is designed for analysis of non-charring ablative materials. This code solves the energy equation, shown below in integral form (Eqn. 1) and includes a term to account for energy convection due to grid motion during ablation. Newton's method is used to solve the energy equation and restarted GMRES [4] is used to solve the associated linearized system of equations. In order to deform the geometry during ablation the mesh is treated as a linear elastic solid and the equilibrium solid mechanics equations are solved. This method has previously been used for axisymmetric ablation problems by Hogan, Blackwell, and Cochran [5], and for fully 3D problems by Dec [6].

$$\underbrace{\int_{cs} \dot{\mathbf{q}}'' \cdot \mathrm{d}\mathbf{A}}_{\text{conduction}} - \underbrace{\int_{cs} \rho h \mathbf{v}_{cs} \cdot \mathrm{d}\mathbf{A}}_{\text{grid convection}} + \underbrace{\frac{d}{dt}\int_{cv} \rho e \mathrm{d}V}_{\text{energy content}} = 0 \tag{1}$$

The material response code is coupled to LeMANS, a hypersonic CFD code developed at the University of Michigan, in order to simulate realistic flight conditions. The coupling is accomplished through an aerodynamic heating boundary condition where LeMANS supplies the material response code with the flow temperature and recovery enthalpy, and the material response returns the updated surface temperature and surface geometry. This coupled simulation approach is applied to the IRV-2 vehicle[7] during its reentry trajectory.

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THERMO-CHEMICAL AND MECHANICAL COUPLED ANALYSIS OF SWELLING CHARRING AND ABLATIVE MATERIALS FOR REENTRY APPLICATION

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One of the major challenges in the design of atmospheric reentry vehicles is the optimization of the thermal protection system (TPS). During a reentry, the vehicle encounter severs heating and mechanical stress. A robust sizing is therefore essential to insure vehicle integrity and the mission success. In order to maximize the payload mass of the vehicle, lightweight charring ablators are commonly chosen as TPS materials for this one shot mission.

To predict the behaviour of the TPS ablative materials under pyrolysis for reentry applications, Astrium ST initiated the development of a specific module of the finite element software SAMCEF: AMARYLLIS. This module uses the Finite Element Method to solve the problem of ablation and thermo-chemical degradation for 1D, arbitrary axis-symmetric or 3D meshes. The numerical model consists of three sets of equations, namely the heat balance equation, the mass balance equation and the charring equations.

In order to enhance the current state of the art for the modelling of thermo-chemically decomposing materials through the integration of swelling behaviour, we used the SUPERVISOR module to elaborate a thermo-mechanical model of intumescing charring and ablative material.

The SUPERVISOR is used as an interface-synchronisation module between MECANO and AMARYLLIS to realize a thermo-chemical and mechanical co-simulation. Current development of an ALE (Arbitrary Lagrangian Eulerian) method and thermal dependencies of the mechanical properties in MECANO allows taking into account various thermo-chemical reacting region and the ablating moving surface in the mechanically swelling behaviour. A global swelling model is built on the basis of various grounds testing such as plasma wind tunnel or IR furnace. The diversity of the experimental environment provided for the robustness of the swelling model. Through this thermo-chemical and mechanical coupling simulation optimal sizing of industrial case become possible.

REAL-TIME ABLATION RECESSION RATE SENSOR SYSTEM FOR ADVANCED REENTRY VEHICLES

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The development of a new sensor system for in-situ, real-time measurements of recession rate of heat shield ablative materials is described. The sensor utilizes a focused ultrasound approach to non-intrusively detect the ablative material's surface loss while simultaneously correcting for acoustic velocity dependencies on temperature. The latter correction is done via an electronic-based scan-focus approach. The multi-source focusing approach is atypical of current ultrasound based sensors used for ablation recession rate measurement, which require a-priori knowledge of temperature distribution within the ablative to yield accurate data on recession rate. The paper describes the development of the sensor system resulting in a brassboard system that demonstrates its operational aspects and possibilities as a heat shield health monitoring system for future reentry vehicles.

METHODOLOGY FOR ABLATION INVESTIGATIONS OF INNOVATIVE ABLATORS IN THE VKI PLASMATRON FACILITY: FIRST RESULTS ON A CARBON FIBER PREFORM

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Following the current developments of a new class of low-density, carbon/resin composite ablators, new efforts were initiated at the VKI on ablation research to understand the complex material response under reentry conditions and to develop and validate new material response models. Promising experimental results were obtained by testing the low-density monolytic composite ablator (MonA) in the 1.2MW inductively heated VKI Plasmatron facility. The application of a high speed camera with short exposure times (2μs) enabled in-situ analysis of both (3D) surface recession and spallation and further made it possible to demonstrate the outgassing effects of pyrolizing ablators. A change in the surrounding gas phase was observed, which is likely due to outgassing products keeping away the hot surrounding plasma before burn-off in the boundary layer. Time-resolved emission spectroscopy helped to identify carbonic species and to capture thermo-chemical effects.

This knowledge was then translated into the development of a testing methodology for charring, low-density ablators in order to investigate the material response in the reactive boundary layer. The successful application of emission spectroscopy encouraged the extension of the setup by two more emission spectrometers for not only temporal but also spatial observations. The extracted experimental data will be employed for comparison with model estimates enabling validation of a newly developed stagnation line formulation for ablation thermochemistry. It was further understood that a proper examination of tested samples has to be performed, especially of the subsurface char layer, which is subjected to ablation. Degradation of the carbon fibers can vary with pressure and surface temperature due to the changing diffusion mechanisms of oxygen that can weaken the internal structure, leading to spallation and mechanical failure. This necessitates ablation tests in combination with microscopic analysis tools (SEM/EDX) for sample examination at the carbon fiber length scale ($\sim 10\mu$m).

Such microscale characterization was recently started at the VKI: A low-density carbon fiber prefom (without phenolic impregnation) was tested in the Plasmatron facility at varying static pressures from 1.5-20kPa at a constant cold wall heat flux of 1MW/m^2, resulting in surface temperatures of around 2000K. Surprisingly, it was found that recession and mass loss of the test specimen was highest at low static pressure (1.5kPa). Furthermore, high-speed-imaging as well as conventional photography revealed strong release of particles into the flow field, probably assignable to spallation.

Micrographs showed that packages of glued fibers (fiber bundles) are embedded in between randomly oriented, individual fibers. It is therefore assumed that ablation of the individual fibers leads to detachment of such whole fiber bundles. It was further found that in an ablation environment of 10kPa ablation lead to an icicle shape on a top layer of 250μm of the fibers with constant thinning, whereas at low pressure (1.5kPa), the fibers showed strong oxidation degradation over their whole length (650μm). Computed diffusion coefficients of atomic oxygen in the boundary layer were more than ten times higher in the case of 1.5kPa compared to 20kPa. This, together with a much lower atomic oxygen concentration at 1.5kPa (decreasing the fiber's reactivity) may allow oxygen to penetrate into the internal material structure. More investigation on both experimental and numerical level is required to confirm those trends. A comprehensive test campaign on a fully developed low-density ablator, ASTERM, is planned for spring 2012 at the VKI.

OXIDATION BEHAVIOR OF CARBON AND ULTRA-HIGH TEMPERATURE CERAMICS USING DYNAMIC NON-EQUILIBRIUM THERMAL GRAVIMETRIC ANALYSIS

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Advanced thermal protection system (TPS) materials that can withstand extreme extreme aerothermal heating loads are needed for use in next generation aerospace vehicles. However, relevant test methods that simulate the flight environment limit our understanding of current and advanced TPS materials. Therefore, the focus of this talk will be to investigate the effect of high temperature gas mixture surface interactions with the oxidation rates of carbon and ultra-high temperature ceramic materials using high temperature thermal gravimetric analysis (TGA) testing methods. We have developed a testing method called, dynamic non-equilibrium (DNE) TGA that allows for us to measure oxidation rates for carbon materials from 600-1600 °C under different partial pressures of oxygen that allow for true isothermal rate data measurement. Our preliminary results for oxidation behavior of carbon-carbon composite and graphite show that with increasing partial pressure of oxygen the oxidation rates follow the same oxidation rate at 1600 °C. At lower partial pressures we observe a deviation from the oxidation rate which is due to the preferential attack of the carbon filler phase in the carbon-carbon composites rather than the fibers. Highly ordered pyrolytic graphite oxidizes preferentially at the edges of the bulk material and a systematic approach to understand bulk oxidation rates for graphite materials is being developed for future use in predictive oxidation rat models based on both oxidation rates and microstructural differences between carbon material forms. Furthermore, we will compare high temperature TGA-DNE and oxyacetylene torch oxidation behavior between carbon materials and ultra-high temperature ceramics which are ideal candidates for sharp leading edge materials that will have to withstand temperatures greater than 2000 °C.

AEROTHERMAL CHARACTERIZATION OF SILICON CARBIDE-BASED TPS IN HIGH ENTHALPY AIRFLOW

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Inductively-coupled plasma generators provide an ideal environment to reproduce the aerothermal heating experienced by a spacecraft re-entering a planetary atmosphere. The flight boundary layer chemistry is duplicated around a TPS model, ensuring a similarity between the flight and ground stagnation-point heat flux.

Experiments conducted in an induction plasmatron on silicon carbide-based thermal protection materials will be described. Several specimens are tested under a wide range of pressure and temperature conditions and investigated by means of infrared radiometry and optical emission spectroscopy. The plasma to which the materials are exposed is characterized in details by calorimetric and Pitot pressure measurements, and numerically rebuilt by means of a nonequilibrium boundary layer model.

The presentation will focus on the thermophysical properties of the material and their dependency on the testing environment. In particular, we will discuss the oxidation features of silicon carbide which are detected both via emission spectroscopy and post-test reflectivity measurements.

GRAPHITE ABLATION EXPERIMENTS IN THE LHEML LASER FACILITY

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Understanding the surface reactions of ablating materials is an important need for modeling Thermal Protection Systems (TPS). There are many experiments out there that capture ablation phenomena seen in hypersonic flows, but ones that can be used to validate Computational Fluid Dynamics (CFD) codes are limited. Most experiments are conducted in arcjet wind tunnels where the enthalpy of the flow is increased by plasma heating due to arc discharges. These flows are hard to characterize due to the unknown dissociated state of the flow that varies spatially along the length of the plasma jet exiting the arc heater. These types of experiments are best for engineering design and not for looking at fundamental physics of surface chemistry. Other options for experimentally measuring surface reaction rates are in ovens or by laser heating of the surface. Laser ablation testing is currently conducted by the Air Force Research Lab Materials Directorate in the LHMEL facility. This work will describe an effort to conduct experiments to be used as validation tools for modeling surface reaction rates.

PYROLYTIC ANALYSIS OF A CHARRING ABLATOR

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The aim of ablation research at Dstl is to understand the key mechanisms which contribute to the behaviour of a charring ablator. Central to understanding the mechanisms and informing the models is knowledge of the chemical products formed during the ablation process and their respective quantities. Following on from David Paynes presentation Mechanistic Analysis of a Charring Ablator at the 4th Ablation Workshop, this presentation describes the approach taken to quantify the pyrolysis products of a charring ablator and the results achieved.

Pyrolytic decomposition of phenolic resin has been performed and a range of analytical techniques have been employed to initially identify, and subsequently quantify, the products:

1. Gas chromatography mass spectrometry (GC-MS) to separate and quantify the volatile aromatic compounds.
2. Gas chromatography thermal conductivity detection (GC-TCD) to separate and identify the permanent gases.
3. Fourier transform infrared spectroscopy (FT-IR) to identify and quantify water and permanent gases.

The products identified included water, hydrogen, methane, carbon monoxide, carbon dioxide, benzene, methylbenzenes, phenol, methylphenols and larger aromatic compounds. Quantitative data is presented demonstrating the composition of the products produced during the pyrolysis of phenolic resin.

A COMBINED EXPERIMENTAL AND MECHANISTIC MODELING APPROACH TO STUDY POLYMER PYROLYSIS

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Motivated by the increasing needs of recovering waste plastics into high-value products or energy, a combined experimental and mechanistic modeling approach was performed to study pyrolysis chemistry of polystyrene, polypropylene, and their mixture. In our work, batch polymer pyrolysis was performed under different reaction temperatures. The detailed product distributions of the pyrolysis experiments were obtained using gel permeation chromatography and gas chromatography equipped with a mass spectrometer and a flame ionization detector. A mechanistic modeling for polymer pyrolysis was constructed separately based on literature parameters and theoretical derivations. Method of moments was used to describe polymer molecular weight distributions, and low molecular weight pyrolysis products were specifically tracked. Our modeling results showed excellent agreement with our experiments, suggesting that the reaction pathways postulated in the model are the major channels responsible for polymer degradation. Our approach can be easily extended to simulate polymer pyrolysis in thermal protection system ablative materials, providing detailed mechanistic understanding of the polymer degradation process for the prediction of the materials response.

STUDY OF MECHANICAL AND THERMAL BEHAVIOR OF POLYMERIC ABLATOR USING MOLECULAR DYNAMICS

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The thermal protection materials used for spacecraft heat shields are subjected to various thermal and me- chanical loads during an atmospheric entry which can threaten the structural integrity of the system. This paper describes the development of a molecular dynamics approach to understand the mechanical and thermal behavior of high temperature polymers. One such material PICA has successfully flown on the Stardust space- craft and is the TPS material chosen for the Mars Science Laboratory (MSL) and SpaceX Dragon spacecraft. Although such polymers have good structural properties at moderate temperature,they became structurally weak at extreme region of temperature and loads. In order to thoroughly understand the response of materials under extreme mechanical and thermal loads it is necessary to investigate atomistic mechanisms of deforma- tion and pyrolysis. MD Simulations are presented to compute the thermal expansion coefficients, stress-strain response,to determine the pyrolysis gas composition entering the char layer from the virgin material, and to identify the main reaction pathways for the interaction between the pyrolysis gases at temperature varying from 500-1500K.

INVESTIGATION OF PYROLYZING ABLATOR IN AN INDUCTIVELY COUPLED PLASMA TORCH FACILITY

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Recent tests conducted in the 30 kW Inductively Coupled Plasma (ICP) Torch Facility at the University of Vermont (UVM) will be presented and discussed. These tests have focused on characterization of the pyrolysis gases emitted during exposure to modest stagnation point heat flux for different plasma gas mixtures. Two sets of test results will be presented. The first comprise tests of PICA samples in nitrogen and air-argon plasma mixtures. Time-resolved emission spectroscopic measurements of the pyrolysis gas injection zone will be discussed. A second set of results will be shown for tests using the pyrolysis gas injection simulation probe developed at UVM to attempt to replicate pyrolysis for longer run times. Again, time-resolved emission spectroscopy results will be used to illustrate the results of this investigation. Results beyond those that were presented at the June, 2011 Thermophysics Conference will be shown at the Ablation Workshop.

ABLATIVE THERMAL PROTECTION SYSTEM STUDY

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Predicting the reliability of the heat shield for crewed space vehicles has been a topic of continuing interest within NASA for many years. The design of a thermal protection system (TPS) is subject to numerous large sources of uncertainty and reliability assessments of such TPS are rare. The proposed talk discusses both the application of Design Of Experiments (DOE) to developing a new arc jet testing campaign for a given TPS and the reliability assessment conducted for the same TPS for a crewed space capsule (similar to Apollo capsules) to withstand re-entry to earth from space.

The objectives of the study were to 1) provide recommendations for a planned arc jet testing campaign, 2) determine the design reliability of a proposed TPS, and 3) conduct a sensitivity analysis to determine the effect of input parameters and user choices on the TPS thermal design reliability. The development of a recommended arc jet test matrix employed a combination of techniques based on the analysis of variance (ANOVA) statistical methodology. The techniques employed include DOE, response surface (RS) methodology and uncertainty quantification (UQ). The recommended test matrix consisted of 30 test cases and includes four replicated condition pairs. Randomization was used to establish the test order, the testing facility, and the test sample cut pattern from three lots of material. The resulting arc jet test matrix was a compromise between one derived from statistical DOE techniques and the existing capabilities of arc jet test facilities located at NASA JSC and ARC. Statistical metrics were employed to objectively compare the assessment-derived matrix to an existing testing proposal. Five of the six metrics examined favored the new proposed test plan over the existing proposed test plan; one of the metrics (and, perhaps, the most important) strongly favored the new test plan proposal over the existing test plan.

The reliability assessment investigated the sensitivity of reliability estimates to various input parameters, which included multiple studies to examine the total bond line temperature reliability based on 7 body point locations for 2 proposed trajectories. Each body point and trajectory combination was subjected to 5 different combinations of trajectory and aerothermal environment assumptions. The reliability was assessed based on a composite material failure criterion, which associated a greater probability of system failure proportional with the exceedance of an assumed safe bond line temperature limit. The study also investigated the sensitivity of reliability predictions to various input and problem formulation parameters. A large, statistically significant difference was found in the estimated TPS reliability when considering various formulations of the reliability problem, including the use of different failure conditions. The proposed talk will summarize the work performed in these areas and highlight some of the findings and recommendations that emerged from the work.

EFFICIENT UNCERTAINTY QUANTIFICATION AND SENSITIVITY ANALYSIS FOR HYPERSONIC FLOW AND MATERIAL RESPONSE SIMULATIONS UNDER INHERENT AND MODEL-FORM UNCERTAINTIES

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Accurate numerical prediction of coupled hypersonic flow fields and ablative TPS material response is challenging due to the complex nature of the physics. The uncertainties associated with various physical models used in high-enthalpy hypersonic flow and material response simulations can have significant effects on the accuracy of the results including the heat-flux and temperature distributions in various layers of ablating TPS material. These uncertainties can arise from the lack of knowledge in physical modeling (model-form or epistemic uncertainty) or inherent variations in the model inputs (aleatory or probabilistic uncertainty). It is important to include both types of uncertainty in the simulations to properly assess the accuracy of the results and to design robust and reliable TPS for reentry or hypersonic cruise vehicles. In addition to the quantification of uncertainties, global sensitivity information for the output quantities of interest play an important role for the ranking of the contribution of each uncertainty source to the overall uncertainty, which may be used for the proper allocation of resources in the improvement of the physical models or reduce the number of uncertain variables to be considered in the uncertainty analysis.

The uncertainty quantification for coupled high-fidelity hypersonic flow and material response predictions can be challenging due to the computational expense of the simulations, existence of both model-form and inherent uncertainty sources, large number of uncertain variables, and highly non-linear relations between the uncertain variables and the output response variables. The objective of this talk will be to introduce a computationally efficient and accurate uncertainty quantification (UQ) and global sensitivity analysis approach for potential application to coupled aerothermodynamics and material response simulations, which is being developed to address the aforementioned challenges. The UQ approach to be described is based on the second-order uncertainty quantification theory utilizing a stochastic response surface obtained with non-intrusive polynomial chaos and is capable of efficiently propagating both the inherent and the model-form uncertainties in the physical models. The non-intrusive nature of the UQ approach requires no modification to the deterministic codes, which is a significant benefit for the complex numerical simulation considered in this problem. The global non-linear sensitivity analysis to be introduced is based on variance decomposition, which again utilizes the polynomial chaos expansions.

In addition to the description of the UQ approach, the talk will also include the presentation of UQ results from a recent demonstration of the methodology, which included the uncertainty quantification and sensitivity analysis of surface heat-flux on the spherical heat shield of a reentry vehicle (a case selected from CUBRC experimental database). This study involved the use of NASA DPLR code and the treatment of the free-stream velocity (inherent uncertainty), collision integrals for the transport coefficients (model-form uncertainty), and the surface catalysis (model-form uncertainty) as uncertain variables. The talk will also include the description of an adaptive UQ framework being developed as part of a NASA JPL STTR project to quantify the uncertainty in multi-physics spacecraft simulations with large number of uncertain variables.

A STATISTICS-BASED MATERIAL PROPERTY ANALYSIS TO SUPPORT ABLATION SIMULATION UQ EFFORTS

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ABSTRACT

Accurate characterization of entry capsule heat shield material properties is a critical component in modeling and simulating Thermal Protection System (TPS) response in a prescribed aerothermal environment. The thermal decomposition of the TPS material during the pyrolysis and charring processes is typically poorly characterized and results in large uncertainties in material properties as inputs for ablation models. These material property uncertainties contribute to large design margins on flight systems and cloud re-construction efforts for data collected during flight and ground testing, making revision to existing models for entry systems more challenging. This work focuses on the following areas of interest to the ablation modeling community: a proper characterization of input probability density functions for material properties, an uncertainty propagation to identify how the uncertainties affect quantities of interest, a sensitivity and uncertainty contributor breakdown, and an analysis of how errors in input characterization contribute to errors in output distributions.

1. INTRODUCTION

For the past half-century there has existed a need to accurately predict in-depth temperatures and surface recession levels for ablative TPS materials to perform design and analysis of entry systems. These predictions are subject to various errors and uncertainties that can be classified into the following categories:

1. *Aleatory* - Uncertainties due to natural variations in the TPS material properties or aerothermal environmental conditions.
2. *Epistemic* - Errors arising from improper input characterization and/or an inability to properly capture the physics of the problem with the ablation model governing equations or numerical methods.

Aleatory and epistemic uncertainties corrupt the accuracy of the predicted outputs and can lead to erroneous conclusions. Expert judgement, experience and good engineering practice mitigate the potential consequences of these uncertainties, but this approach falls short when the system design, aerothermal environment and entry trajectory deviates from established practice.

Over the past decade, numerous analyses have been performed using a probabilistic interpretation of aleatory uncertainty. Monte Carlo methodologies have been applied to uncertain parameters in ablation[9, 6, 17] and aerothermal[2, 3] models, to determine the effect on imposed heating, subsurface temperatures, surface recession levels and other quantities of interest. These approaches have given rise to new methods for assessing TPS margin[8] and have been the basis for new design and risk assessment methodologies. However, as is the case in deterministic simulations, the outputs from stochastic analyses depend strongly on the characterization of the input distribution(s). In the ablation modeling community, little work has been performed to collect and analyze the available material property data to arrive at appropriate input distributions that capture the correct trends and relationships between material properties. In the works cited, all Monte Carlo analyses are performed assuming independent gaussian random variables as inputs with distribution parameters (μ and σ) determined by expert opinion. This particular prescription of input functional type can lead to improper and non-physical inputs to the ablation models. Furthermore, there has been little quantitative analysis to determine how the assumed input PDF shapes affect the shape of the output PDF and any corresponding conclusions on reliability and margin.

This work addresses some of the highlighted shortcomings in the existing body of work for uncertainty quantification efforts for ablation simulations. Primary goals are outlined below:

1. *Construct a revised set of input material property PDFs for modern TPS materials.* Known dependencies exist between material properties (density, thermal conductivity, specific heat, etc.) and should be appropriately treated in non-deterministic analyses. A prescription of the functional type of the input PDF is to be avoided and instead will be based on a Kriging fit to available experimental data. Results from NASA's Mars Science Laboratory (MSL) TPS design and MSL Entry, Descent and Landing Instrumentation (MEDLI) material property testing efforts form the database for the analysis.

2. *Propagate input uncertainties to output quantities of interest, perform model sensitivity analysis and rank the primary uncertainty contributors.* The propagation analysis determines the effect of the revised input set on typical quantities of interest, including in-depth temperature, bond line temperature, and recession depth. The model sensitivity study is performed using standard finite-difference methods while uncertainty contributors are determined by calculating correlation coefficients and Sobol indices.

3. *Characterize the errors output PDFs as functions of the quality of the input distributions.* A quantitative assessment of the affect of additional material property data on output error reduction is performed. A specified number of samples taken from the input PDFs generated in (1) (assumed to be "truth" distributions) are used to create approximate input distributions to be used in a Monte Carlo ablation analysis. Output PDFs from the approximate models are compared to "true" output PDFs on the basis of Kullback-Liebler divergence. This framework establishes a mapping between the number of samples used to generate the approximate inputs and the error in the predicted outputs.

The ablation analysis is performed using the Fully Implicit Ablation and Thermal Response Program (FIAT)[5] developed and used by NASA to perform analysis and design for flight systems.

2. PRELIMINARY RESULTS

The ablation simulations in this abstract are calculated in aerothermal environments anticipated for the Mars Science Laboratory during the entry phase of its mission, scheduled for the summer of 2012. The sensitivity study was performed at two locations on the heat shield corresponding to embedded instrumentation, called MEDLI Integrated Sensor Plugs (MISPs). Each plug has four in-depth thermocouples (TCs) that will track the evolution of temperature through the TPS during entry.

The finite-difference sensitivity analysis for MISP locations 3 & 4 at each thermocouple locations are shown in Fig. (1) and Fig. (2) respectively. The stacked-area plots show the relative sensitivity of the TC temperature to the 11 material property inputs to FIAT. For a given vertical slice along the x-axis, the fraction of color belonging to parameters indicate how significant those parameters are at that time step. For an example, see Fig. (1a). The sensitivity of TC1 temperature at MISP 3 to char density is zero until the onset of char formation 33 seconds past entry interface where it then contributes significantly to the sensitivity of the TC reading. Note the time axis on Fig. (1a) differs from the other subfigures due to the burnout of the thermocouple as the TPS material recedes beyond its in-depth location in the plug.

In anticipation of true TPS material property data, preliminary uncertainty propagation has been performed using fictitious input distributions. This propagation has been performed with independent gaussian and uniform random variables as a placeholder for more accurate input distributions that will be characterized for the final work. Propagation analyses of 2000 FIAT runs for each distribution type each are shown in Fig. (3) at MISP 3. TC mean values for each time step are shown in solid lines and a band of two standard deviations is enclosed in the dotted lines.

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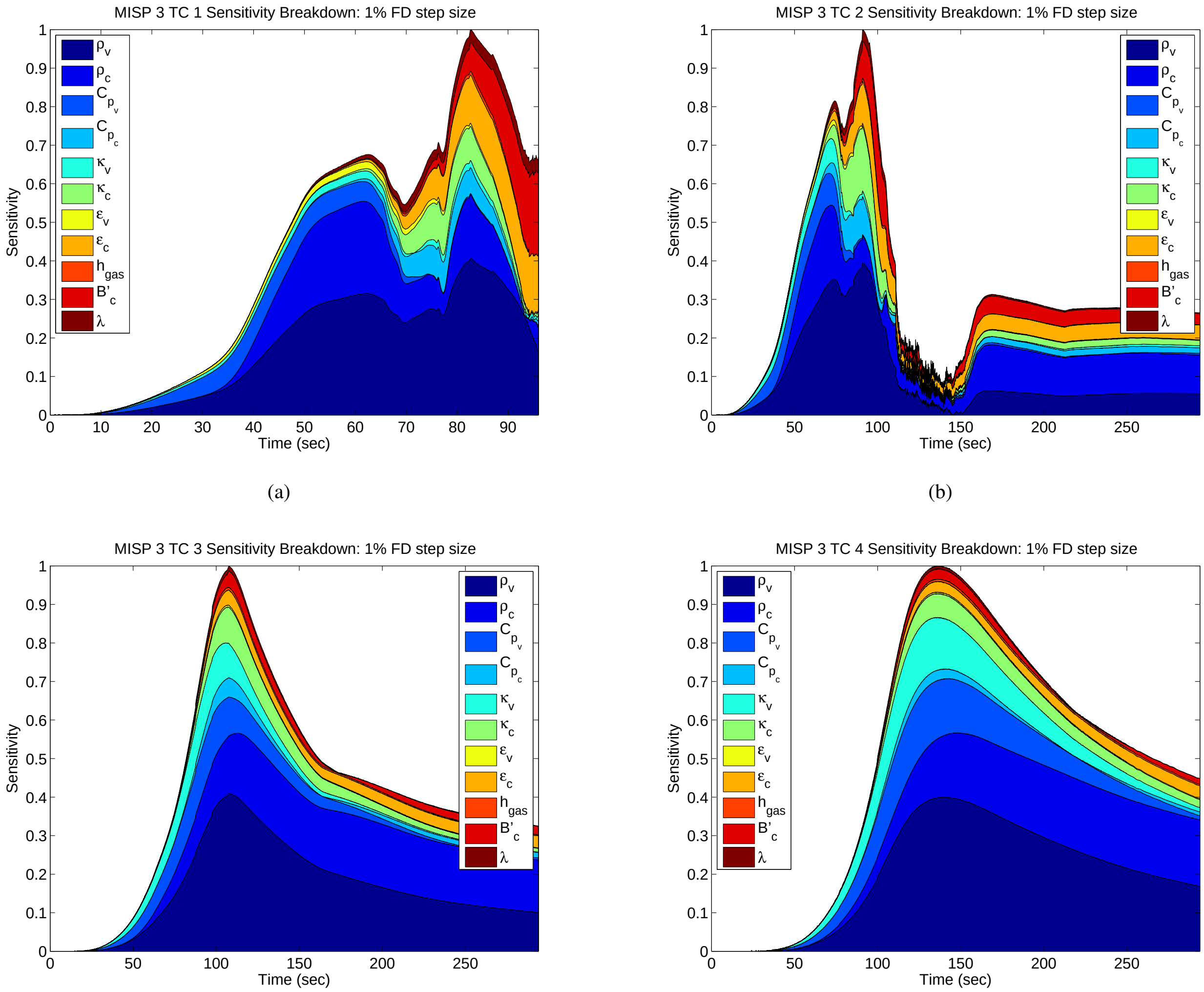

(a) (b)

(c) (d)

Figure 1: MISP 3 Finite-Difference Sensitivity Analysis.

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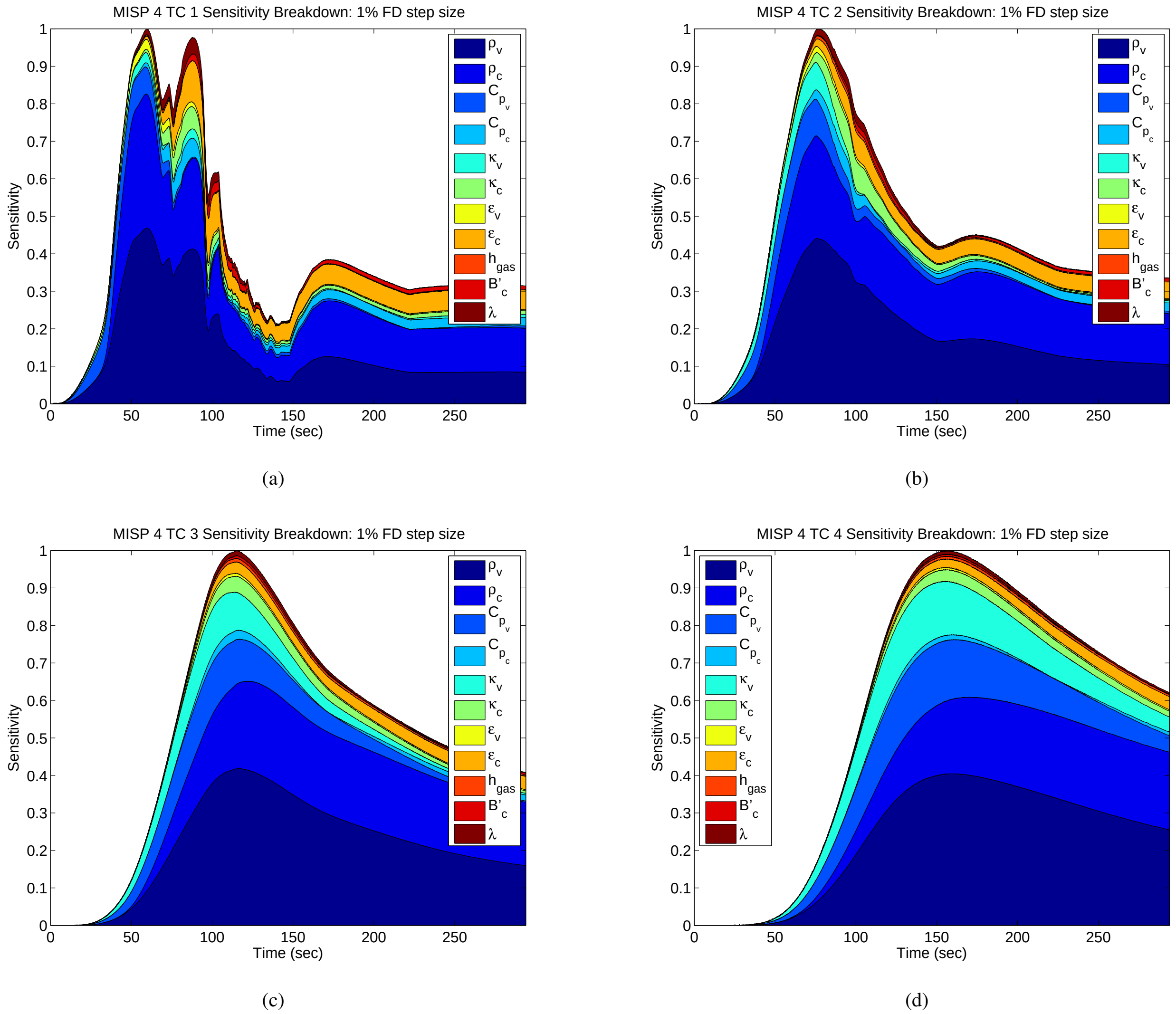

Figure 2: MISP 4 Finite-Difference Sensitivity Analysis.

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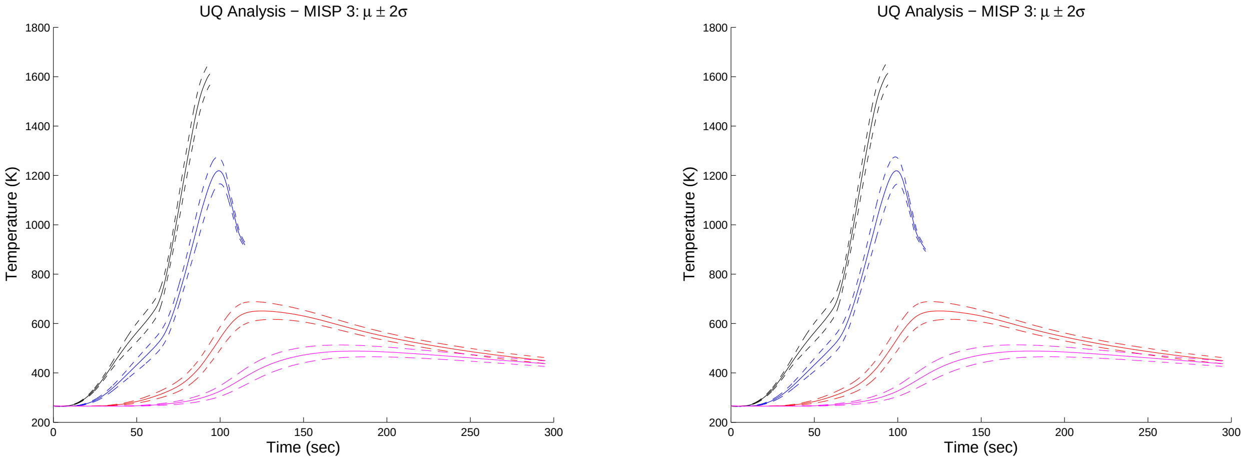

(a) Normal Distributions (b) Uniform Distributions

Figure 3: MISP 3 Uncertainty Quantification Analysis Using Differing Input Distributions.

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3D MICROSTRUCTURAL CHARACTERIZATION OF MATERIALS

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Thermal protection systems are commonly comprised of composite materials, often with highly anisotropic micro/meso-structures. The heterogenous and anisotropic nature of the TPS materials can lead to significant thermal residual stresses at both room and high temperatures and complex deformation mechanisms. Three-dimensional characterization of material microstructures may provide important inputs modeling of both thermal residual stresses and deformation mechanisms.

Modern characterization techniques allow for direct three dimensional imaging of both as-processed and deformed materials at scales ranging from centimeters to nanometers, with the resolution of some applications approaching sub-nanometer. For example, electron tomography can reproduce 3D structures with nanometer resolution, though the field of view is limited to microns. Conversely, neutron diffraction can reproduce objects of many centimeters in size with a resolution (voxel size) of about 100-150 μm.

Analysis of deformed materials is generally more difficult, as contrast in signals between pristine and deformed materials is not always adequate. However, a number of characterization techniques may be utilized to analyze deformation mechanisms in two or three dimensions. These deformation mechanisms may then serve as inputs for material modeling, though accurate modeling of complex material system is non-trivial and generally requires significant computing power. Multiple case-studies will be discussed relating to modeling of experimental microstructures and direct two and three-dimensional imaging of deformation mechanisms.

ULTRASONIC THERMOMETRY FOR RECESSION MEASUREMENTS IN ABLATIVE MATERIALS

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Recent developments in ultrasonic instrumentation & sensors, improved signal processing, and high speed data acquisition have rekindled interest in ultrasonic thermometry and made temperature localization feasible and economically attractive to a wider range of applications. Ultrasound-based temperature measurements offer several advantages: they are non-intrusive, have high temporal response, isolate the sensor from explosive or chemically harsh environments and do not adversely influence thermal transport. Ultrasonic thermometry techniques rely on precise measurements of ultrasonic time-of-flight (ToF) which forms the basis for many applications including measurements of flow, heat flux, temperature, ablation and strain. In this report, we characterize the ultrasonic propagation characteristics of several ablative materials. Properties relevant to ultrasonic thermometry include backscattering properties, attenuation coefficient, ultrasonic velocity, and velocity-temperature coefficient. We will present preliminary experiments directed at developing ultrasonic methods for simultaneous temperature and recession measurements on ablators. Various approaches to measuring recession, heat flux, and internal temperature profiles in ablators will be described.

ON THE MODELING OF HIGH-SPEED TURBULENT FLOWS WITH APPLICATIONS TOWARDS REENTRY ABLATION

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The fluid dynamics of an ablating hypersonic turbulent boundary layer is a complex process with strong coupling to the surface response. The overarching objective of our research is to improve the accuracy of turbulent heat flux and shear stress modeling for this class of flow. Our approach is to first establish physics based transport equation frameworks for model development, and then perform model driven experiments to isolate underlying phenomena. Among the complications is roughness and streamline curvature induced mechanical non- equilibrium. In this presentation, a description of a recent Mach 5 experimental campaign focused on characterizing the role of these complications on the Reynolds stresses is given first. This is followed by a discussion of the impact on modeling and control. The results from the study are encouraging from the perspectives that (1) existing Reynolds stress transport and large-eddy methods show promise in capturing the observed processes provided suitable understanding of the turbulence structure is achieved and (2) the mechanisms appear controllable.

AN ADJOINT METHOD TO DETERMINE THE EFFECTIVE MATERIAL PROPERTIES OF AN ABLATOR

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The determination of the effective thermal properties of a material from thermocouple data has always been very labour intensive. Similarly determining the Arrhenius parameters for a decomposition model from thermo-gravimetric analysis is also very time-consuming. There is little formalisation of the procedures used to determine the material properties. Despite the fact that some effort has been devoted to this topic in the literature, it is not clear whether comparable effective material properties data would result if several groups used the same experimental data. The FGE Ablation code FABL has been written in an adjoint form and has successfully been used to efficiently determine the effective material properties from experimental data. The method provides a formalised procedure where the iterative aspect of this process has been automated.

The adjoint form of FABL calculates the partial differential of a cost function to many input variables in one pass of the code. The Jacobian (a matrix of the gradients) can be compiled in one calculation for n input variables, instead of from n+1 calculations which would be needed if it was calculated numerically. The Jacobian can then be used to optimise the input parameters and minimise the cost function. The cost function used in FABL is simply the sum of the absolute relative difference between the measured and predicted results. This can be the difference in thermocouple and/or surface temperatures or the variation of density with time, depending on the case being run. A simple steepest descent optimiser is currently the preferred optimisation method. The structure and flow of information in FABL Adjoint is shown in Fig. 1.

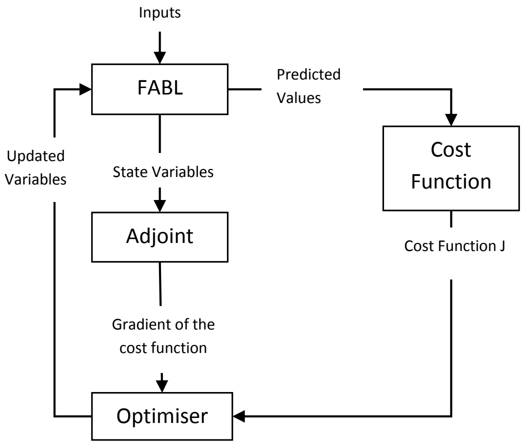

Figure 1: Overall Structure of the FABL Adjoint

The ability to calculate the Jacobian quickly and efficiently means that many material properties can be optimised in a relatively short amount of time without the need for large computations or many man hours. Many experimental data sets for the same material can be compared at once and material properties can be derived to best fit all the available experimental data. The data does not have to come from the same experimental campaign.

The adjoint has advantages when determining properties for a new material or supporting physics updates to the model. Effective material properties are only applicable for the experiment and model they are derived from. The adjoint allows the effective properties to be easily updated when the model is developed and extended or new experimental data becomes available.

INVESTIGATION OF BLOWING EFFECTS ON TURBULENT FLOW OVER A ROUGH SURFACE

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Entry of spacecraft into an atmosphere occurs at hypersonic speeds, generating extremely complex flow fields, with aerothermodynamic effects which can cause the surface to be subjected to extreme heating. It is therefore important to protect the vehicle and its payload using a thermal protection system (TPS). Heat shields, which are an important part of a TPS, can be of either ablative or non-ablative types. For an ablative TPS, the energy is dissipated through surface material charring and ablation, as well as releasing gasses which serve to carry energy away from the TPS and thus reduce the total heat flux into the vehicle.

One of the many difficulties with designing such a system is accurately modeling the flow physics near the TPS surface itself. One important consideration is the state of the boundary layer forming over the surface which, if it has transitioned to turbulence, can drastically increase the transport of mass, momentum and energy. In addition, as an ablative TPS pyrolyzes, the surface will become rough and pyrolysis gasses will be injected into the flow, which can potentially alter the structure and organization of the turbulence over the TPS surface. Understanding the behavior of wall-bounded turbulence under these conditions can benefit modeling of the near-wall flow phenomena critical in designing and optimizing an ablative TPS.

Figure 1: Blowing rig in place on test section of turbulent channel flow facility.

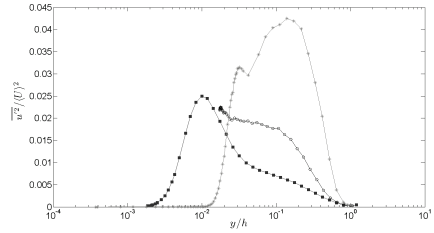

Figure 2: Comparison of turbulence intensity as a function of normalized wall distance for the: smooth walled case (-■-), the rough walled case (-○-) and the rough walled case with flow injection (-*-).

The current effort investigates the fluid dynamics of a turbulent wall layer over a rough surface subject to additional momentum injection through the surface, which is intended to represent the conditions experienced by an ablative TPS when the near-wall flow has transitioned to a turbulent state. The current research seeks to understand the effects and interaction of both surface roughness and flow injection on a turbulent wall layer. Experiments are currently underway which utilize a turbulent channel flow facility and a specialized blowing apparatus (pictured in Fig. 1) used to inject flow through the geometrically simple, sinusoidal, quasi-2D, rough surface. Measurements are being made of the wall-normal dependence of the streamwise component of velocity using hot-wire anemometry.

Figure 2 shows the wall-normal dependence of the streamwise Reynolds stress for a smooth-walled case, a case with surface roughness and a case with both surface roughness and momentum injection, at matched Reynolds number. These results indicate a significant impact of both the roughness and combined roughness-and flow injection when compared to the baseline smooth-walled case. As expected, the additional roughness increases the Reynolds stress further away from the wall. More interestingly, the addition of momentum injection is found to shift the near-wall peak away from the surface, as well as producing a second peak in the outer- scaled region, indicating a strong modification of the turbulence production cycle within the wall-layer. Ongoing work is being performed to examine the spectral content of the turbulence as well as the influence of the momentum-injection to bulk velocity ratio on the turbulence structure.

NUMERICAL INVESTIGATION OF THREE-DIMENSIONAL EFFECTS WITHIN A CHARRING ABLATOR

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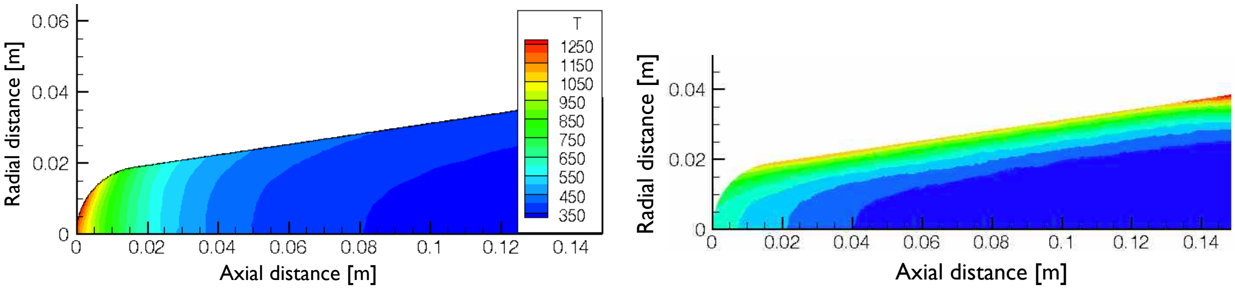
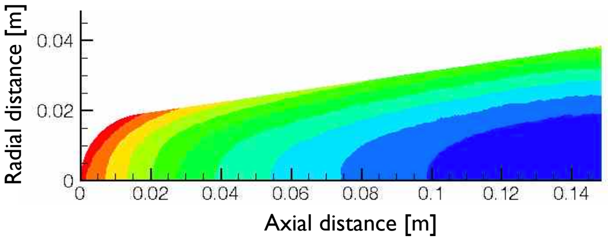
Re-entry of a spacecraft occurs at hypersonic regime where flow field is extremely complex. High temperature gradients occurring in the shock-layer region ionizes and dissociates the air. Even if a large portion of heat generated during this process is convected away in the surrounding air, a fraction of it is still transferred to the vehicle. Therefore, it is important to protect the vehicle with a suitable kind of shielding. Of many techniques available today, the use of ablator material is increasing in popularity. The basic idea behind an ablating heat shield is that the energy incident on the spacecraft is used to vaporized the material, thus preventing a significant part of heat to be transferred into the structure. Available literature indicates that most of the past investigations either do not consider the actual physical processes taking place during ablation, or are limited to a one-dimensional model. The present communication shows the development of a numerical model for simulating the multidimensional heat transfer phenomena that occurred in a typical ablative TPS. Figure 1a) illustrates the computed temperature distribution for the IRV-2 vehicle after 4 seconds of constant exposure. As expected, maximum levels of temperature is observed at the blunted nose section of the body. A gradual decrease in temperature values is also apparent as one move towards the base section. Figure 1b) to c) illustrates the same results while using different values of an anisotropic thermal conductivity. As can be seen, the results are significantly different. These results illustrates the first steps of an ongoing project to develop a comprehensive multiscale, multi-physics and multi-dimensional material response code aimed at modeling charring and surface ablators.



(a) Isotropic thermal conductivity of $k = 50$

(b) Anisotropic Thermal conductivity of $k_{xx} = 5$ and $k_{yy} = 50$



(c) Anisotropic Thermal conductivity of $k_{xx} = 50$ and $k_{yy} = 5$

Figure 1: Temperature distribution within the IRV-2 vehicle after 4 seconds of exposure.

DST-SHELLS USED AS AN ABLATIVE MATERIAL

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Deep Springs Technology (DST) manufactures hollow shells made of Silicon Carbide. These shells are lightweight and strong, and posses great heat conducting properties. DST has just begun to work with companies who are considering our shells as an ablative material.

ADVANCED THERMAL PROTECTION SYSTEMS (TPS) AND TRANSITION ANALYSIS: UNIQUE EXPERIMENTAL CAPABILITIES AND CURRENT RESEARCH EFFORTS AT THE UNIVERSITY OF TEXAS AT ARLINGTON

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A unique experimental capability in the academic panorama is the *1.6* MW-class arc-jet facility located at the *A*erodynamics *R*esearch *C*enter of the University of Texas at Arlington. The arc- heated wind tunnel has recently been refurbished and repurposed (extended testing time of the order of minutes and testing gas-composition control) for the study and characterization of the aerothermal response of TPS candidate materials for sustained hypersonic flight.

The newly modified facility has been extensively used to support two recent screening and characterization projects for *C*arbon-*C*arbon *A*dvanced *T*echnologies (*C-CAT*): a material characterization for the *SWEAP* program sponsored by *ONR* and a project on advanced TPS sponsored by *AFRL* (ITAR- restricted technical data).

A detailed characterization of the high-enthalpy plume is being performed with a null-point calorimeter obtained from NASA Ames Research Center. Tests with a TEFLON probe are planned to investigate the uniformity of the flow for selected configurations.

Current research interests include the study of the effects of finite Damkohler number on supersonic transition over realistic surfaces in active and passive oxidation regimes. The emphasis is on the analysis of transition bypass over axisymmetric geometries.

A separate study is focused on novel applications of transpiration cooling for C-C/SiC materials. The experimental investigation will leverage on *IR thermography* and *spectroscopy* to examine the effects of transpiration on the material response of a test article subjected to the high enthalpy flow. To accommodate specific properties of the fluid medium used in transpiration, the carbon- carbon TPS material will require custom tailored values of porosity.

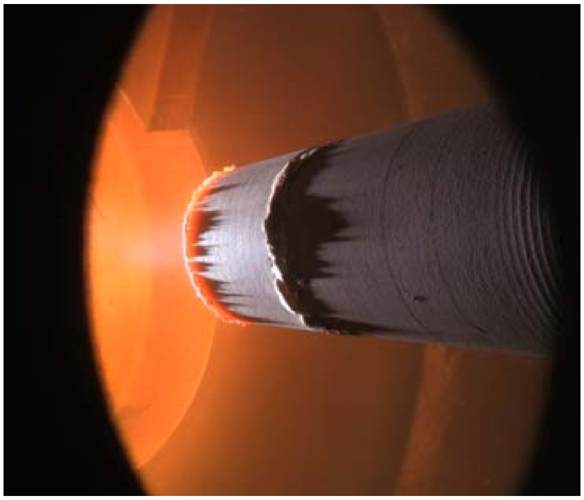

Figure 1: Material article during arc-jet testing (UTA Arc-Heated Facility)

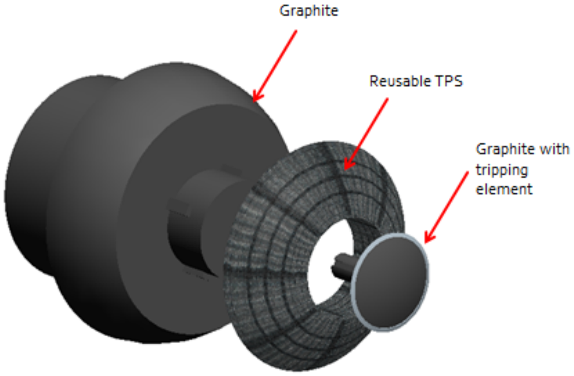

Figure 2: Bypass transition with tripping elements

DEVELOPMENT AND VALIDATION OF SACRAM: A SWISS APPROACH TO THE COMPUTATIONAL RESPONSE OF AN ABLATIVE MATERIAL

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Future space exploration missions foresee high-speed entries into planetary atmospheres. These latter imply extreme thermal conditions to which the space vehicle is exposed to, and require an appropriate thermal protection system (TPS). The interest of the scientific community in modelling and testing of materials that compose the TPS has hence greatly increased over the past few years. Since a complete set of material properties is not available in open literature, it is difficult to numerically rebuild experiments. The inter-code comparison exercise proposed by the AF/SNL/NASA Ablation Workshop aims to give a baseline platform for ablation code calibration, with a complete set of material and gas properties.

SACRAM 1.0 is a one-dimensional, finite-volume code that solves transient mass and energy continuity equations for a carbon-resin composite material that undergoes pyrolysis and charring. Mass loss is calculated integrating Arrhenius laws, with the hypothesis that all decomposed solid material is transformed into gas, and no closed pores appear. The solid mass conservation law translates therefore in a conservation of the porosity. Darcys law is used in the momentum conservation equation to determine gas velocity in the pores. Time integration is performed with an implicit method, and non-linarites are treated with NewtonRaphson iterations. Thermal non-equilibrium between gas and solid phases, formulation of pyrolysis gas as a multi-species entity and internal radiative heat transfer are under development and will be implemented in SACRAM version 2.0.

SACRAM will also help to increase European scientific interest and activity in the field of ablation, where currently US presence in primary. In fact in the session dedicated to this exercise at the 4th AF/SNL/NASA Ablation Workshop (1-3 March 2011, Albuquerque, New Mexico), out of the fourteen research groups that presented their results, only two were from European countries.

COMPUTATION OF SURFACE CATALYSIS FOR GRAPHITE EXPOSED TO HIGH-ENTHALPY NITROGEN FLOW

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The high temperatures on a hypersonic vehicle surface caused by heat loads encountered during (re-)entry through a planetary atmosphere require a reliable Thermal Protection System (TPS) that makes a good understanding of the physical and chemical processes essential for its design. Surface catalysis is a crucial chemical process that directly impacts aerothermal heating of the vehicle TPS. The effects of surface catalysis for graphite exposed to high-enthalpy nitrogen flow are examined in this study.

The objective of this study is to investigate and implement surface chemistry models to describe dominant gas-surface processes. As a first step, a binary catalytic atom recombination model is implemented in the Michigan Aerothermodynamics Navier-Stokes computational fluid dynamics (CFD) code LeMANS, developed at the University of Michigan. It is a general purpose, parallel, three-dimensional code that solves the laminar Navier Stokes equations including chemical and thermal nonequilibrium effects on unstructured computational grids. In LeMANS, prior to the present work, wall catalycity effects were accounted for by choosing a non-catalytic or a super-catalytic surface as the species boundary condition. The full range of catalycity regimes, from a non-catalytic wall to a fully- catalytic wall can be simulated by using the binary catalytic atom recombination model. The entry flight environment considered is the post shock subsonic high enthalpy gas flow. Assessment of the computations is performed using experimental tests that were conducted in the 30 kW Inductively Coupled Plasma (ICP) Torch Facility at the University of Vermont. It is designed to test scaled material samples in high enthalpy gas flows for simulation of planetary entry and Earth atmosphere re-entry trajectory heating conditions. The comparative analysis of the computed profiles of gas temperature and relative nitrogen atom density with the experimental results is performed. The free stream conditions and wall temperature used are based on the experimental set up and are provided in Table 1.

Table 1: Freestream and wall boundary conditions

Mach Number	Temperature	Density	N_2 Density	N Density	Wall Temperature
M_∞	T_∞ [K]	ρ_∞ [kg/m^3]	$\rho_{N_2\infty}$ [kg/m^3]	ρ_{N_∞} [kg/m^3]	T_w [K]
0.11	7000	3.36×10^{-3}	0.35×10^{-3}	3.01×10^{-3}	1590

The equilibrium composition of nitrogen gas mixture at the inlet for the given temperature and pressure are calculated using the NASA program Chemical Equilibrium with Applications (CEA). The influence of different flow physics assumptions viz. thermal equilibrium, thermal nonequilibrium and thermochemical nonequilibrium and surface catalysis (non-catalytic and fully-catalytic surface) on the numerical solution is studied. The main calculated parameters analyzed are translational temperature, relative nitrogen atom density, and surface heat flux. The results from simulations showed that thermal nonequilibrium effects are negligible and that the flow studied is in a state of weak thermochemical nonequilibrium. Strong surface catalysis effects on the boundary layer gradients of temperature and species concentration, and heat transfer to the surface are observed. A fully catalytic surface caused the heat flux to increase by a factor of approximately 3.5 as opposed to a non-catalytic surface for thermochemical nonequilibrium.

COMPUTATIONAL CHEMISTRY MODELLING OF THE OXIDATION OF HIGHLY ORIENTED PYROLYTIC GRAPHITE

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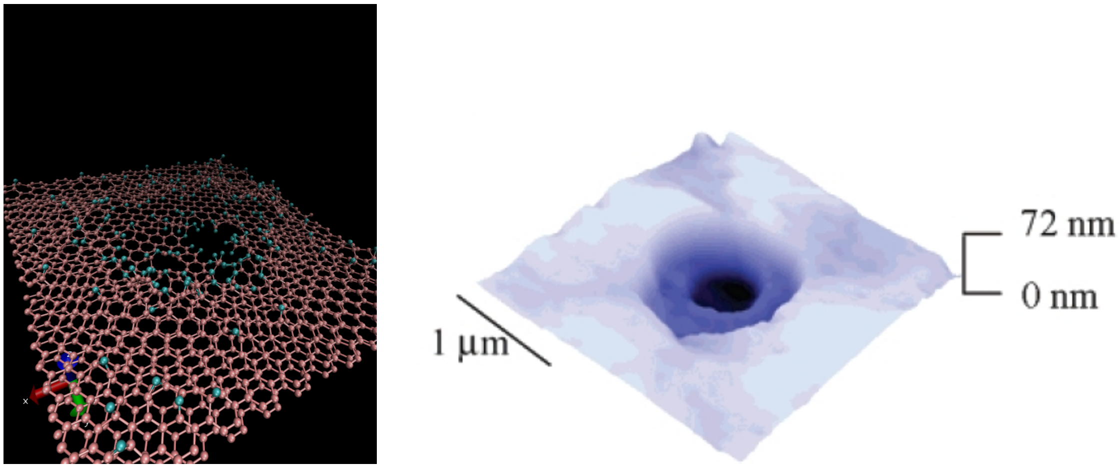
Under high heat flux, carbon based Thermal Protection Systems (TPS) are observed to rapidly ablate and an accurate characterization is essential to their design. Dissociated oxygen atoms (from the gas phase) striking the surface of TPS could lead to several possibilites. The O atom could adsorb on the surface, recombine with another O atom to form O_2 and oxidize the surface to produce CO or CO_2 resulting in recession of the surface (ablation). The goal is to predict finite rate models for these reactions which could be incorporated into CFD and DSMC solvers. Our efforts are to predict the rates through large scale Molecular Dynamics (MD) simulations using the ReaxFF potential which enables accurate simulation of large chemically reacting systems of molecules. In this work, we simulate the collision of hyperthermal (5eV) O atoms on Highly Oriented Pyrolitic Graphite (HOPG) at 525K. The simulations are compared to molecular beam experiments performed by Minton[1] and co-workers.

The simulations predict the pit growth in the intraplanar direction to be much more rapid than etching in the interplanar direction. This was observed experimentally (Fig. 1) where shallow but wide etch pits were created. The experimental results predict the probability of oxidation (removal of carbon atom) in the prismatic plane (intraplanar direction) at about 0.44 (roughly 1 carbon atom for 2.3 O atoms) and our results predict that about 1 carbon atom is removed for every 5.96 O atoms. The simulations have reasonable quantitative and qualitative agreement with experimental results. Results of the surface temperature dependence on etching rate will also be presented.



(a) Surface of HOPG after O atom collisions from simulation. Only top 2 layers shown

(b) Surface of HOPG after O atom collisions from experiments

Figure 1: The figure compares the surface of HOPG after collisions with O atoms at 5 eV from both simulations and experiments.

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DYNAMIC NON-EQUILIBRIUM THERMAL GRAVIMETRIC ANALYSIS OF OXIDATION RATE MEASUREMENTS FOR ULTRA-HIGH TEMPERATURE CERAMICS UP TO 1600°C

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During hypersonic flight, vehicles need materials such as ultra-high temperature ceramics (UHTCs) for thermal protection system in order to withstand temperatures greater than 2000°C; therefore, understanding the oxidation behavior of these materials is important. We examine oxidation behavior of ZrB_2-SiC composites by investigating the ratio of total specimen edge length to total specimen surface area and determine its relevance for developing reliable oxidation methods. We also investigate dynamic non-equilibrium thermogravimetric analysis (DNE TGA), which differ from conventional oxidation rate measurements by not including mass changes from heating and cooling. This method of DNE TGA is used to oxidize UHTCs and carbon to obtain isothermal rate measurements from 1000-1600°C and 0.29-19 kPa pO_2. We determine, for reliable data, specimen parts with ratios less than 0.5 should be used for oxidation testing due to the reduced effect of edge and corner oxidation compared to bulk oxidation for UHTCs. Isothermal *in situ* mass measurements follow similar trends with temperature for DNE TGA; with increasing temperature, overall mass gains increase for UHTCs. Pressure dependence of DNE TGA results in mass gain from 8.9-19 kPa pO_2 and mass loss from 0.29-2.0 kPa pO_2 for UHTCs.

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