A pyrolysis and ablation toolbox based on OpenFOAM

- with application to material response under high-enthalpy environments

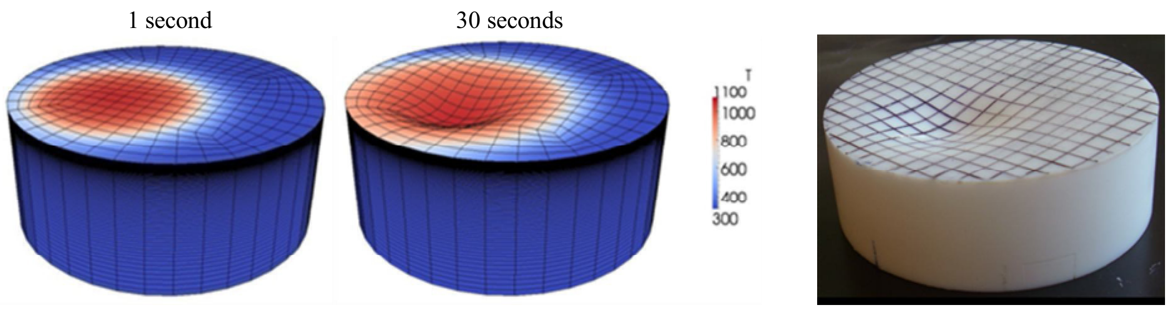
Dr. Jean Lachaud, jean.r.lachaud@nasa.gov **Dr. Nagi N. Mansour**, nagi.n.mansour@nasa.gov	NASA Ames Research Center 94035, Moffett Field, CA, USA

Abstract

A critical problem in the design of Thermal Protection Systems (TPS) for planetary probes and re-entry capsules is the choice of a heatshield material and its associated material response model. Typically, in Earth re-entry, the temperature of the flow reaches 10,000K in the shock layer and leads to a wall temperature of about 4000K. No (known) material is able to withstand such conditions. For very high speed entries, a new class of ablative materials has been introduced and validated in flight by the Stardust (1) mission [1]. This new class of low density Carbon/Resin (C/R) composites, made of a carbon fiber preform impregnated in phenolic resin, is rapidly developing. PICA [2], the low density C/R conceived at NASA Ames and used for Stardust, has been selected and adapted for Mars Science Laboratory (MSL) heatshield. PICA-X has been developed by SpaceX (Space Exploration Technologies Corp.) with the assistance of NASA to protect their Dragon capsule during re-entry [3]. The European Space Agency (ESA) is currently supporting the development of a light weight C/R ablator that could be used for sample return missions [4]. Under a certain number of conservative hypotheses, state-of-the-art pyrolysis-ablation models may be used to design TPS made from this new class of PICA-like materials. However, revisiting the state-of-the-art pyrolysis-ablation models appears crucial to improve current design tools [1, 5] and to understand, estimate, and reduce design uncertainties [6]. Therefore, numerous conservative hypotheses have to be removed; this dramatically increases the complexity of the models. We are developing a modular Pyrolysis-Ablation Toolbox that will enable engineers to test new models without having to go through equation discretization and hard coding. A high level formalism may be used instead. Equations may be written in a top-level solver in their mathematical form. Relevant finite-volume schemes and solvers are chosen at execution time. OpenFOAM open source CFD software package is used as a framework to produce this modular Pyrolysis-Ablation Toolbox. As an illustration, the simulation of the ablation of a Teflon cylinder is shown in Fig. 1.

1- Short description of the physics

During re-entry, a fraction of the heat is transferred to the TPS leading to a gradual temperature increase of the material (Fig. 2-a). The low density C/R composites are made of a fibrous carbon preform impregnated in phenolic resin (Fig. 2-b). The residual porosity is about 85%. With the temperature increase, the virgin material is successively transformed (and destroyed) by two phenomena [7]. The first transformation phenomenon is called pyrolysis. During pyrolysis, the phenolic resin progressively carbonizes into a low density carbon and loses around 50% of its mass, producing pyrolysis gases. The pyrolysis gases are transported out of the material by diffusion and convection through the pores. During this transfer, their chemical composition evolves as their temperature increases and as they mix with air that diffuses into the pores of the material from the boundary layer. The second transformation phenomenon is the ablation of the char that is composed of the fibrous carbon preform and carbonized phenolic resin. Depending on re-entry conditions, ablation may be due to heterogeneous chemical reactions (oxidation, nitridation), phase change (sublimation), and/or mechanical erosion (spallation). Material response models should predict accurately the ablation rate and the peak temperature of the bondline at the interface of the TPS and the substructure.



a) Simulation using OpenFoam (Temperature in °C) b) Picture of the sample after test (30 s)

Fig. 1- Ablation of a Teflon cylinder, 1MW/m², 30 seconds, NASA Ames X-Jet (off-centered)

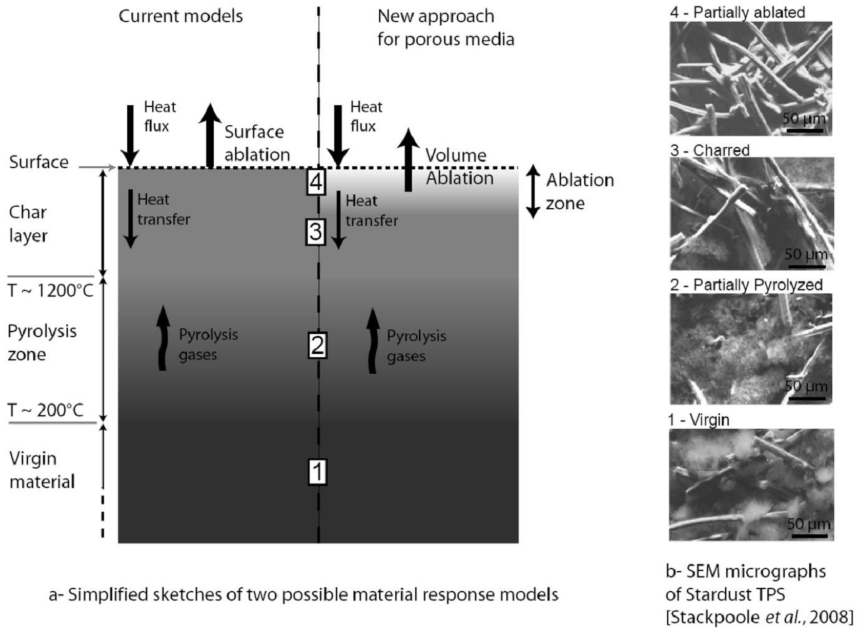


Fig.2. Material response to a re-entry heat flux

2- State-of-the-art models

The models currently used for design are inspired from the model of Kendall et al. published in 1968 [7]. They are based on five major assumptions: 1) pyrolysis gases are frozen until they reach the flow field; 2) pyrolysis gases are transported by convection only; 3) air does not penetrate inside the material; 4) ablation only occurs at the surface; 5) the solid at the surface is in chemical equilibrium with the gas. In other words, from the extremely complex phenomena occurring in a porous ablative material, only Fourier's heat transfer and the pyrolysis of the solid are modeled [7]. Interestingly, this simplified model has been able to reproduce within a reasonable accuracy Arc Jet tests carried out on PICA in conditions relevant to the re-entry of NASA's Crew Entry Vehicle (CEV) [8]. However, the limits of the model have been recognized when compared to other test cases. In conditions relevant to the Mars Science Laboratory (MSL) mission, the CEV model did not work well. In order to achieve satisfactory agreement, the heat transfer coefficient had to be modified to approximate the experimental data [9]. The modifications to the heat transfer coefficient are needed to account for the phenomena that are not modeled (enthalpy of the chemical reactions, mass transfer, and complex pyrolysis laws). Another well known shortcoming with current models is the overestimation of ablation rates because equilibrium chemistry is an upper-bound model (compared to possible finite-rate chemistry). Stardust post-flight analyses have shown that the recessions near the stagnation point was overestimated by 61% using equilibrium chemistry [1]. Finite-rate chemistry models have been proposed and implemented to improve the accuracy of current models [11], with a better fit to the experimental data being obtained. However, the approach proposed in ref. [10] lacks several important mechanisms (*e.g.,* penetration of oxygen in the material, chemistry of the pyrolysis gases).

3- New developments using OpenFoam

A complete analysis and modeling of all the phenomena and of their coupling is necessary in order to develop a reliable model. These new developments can be summed up in a 6 step code-development strategy:

0- Reproduce state-of-the-art-ablation codes. The first module, PAT-0, has been validated against state-of-the-art pyrolysis ablation codes. It is implemented in 3D, while current design tools are 1D or 2D axi-symmetric. The surface recession is handled using the OpenFoam moving mesh library. The surface recession velocity is deduced either from a surface temperature law (new dynamicFvMesh class), or from state-of-the-art equilibrium ablation tables [7]. A table reader and a four dimension interpolation class have been written to import the equilibrium tables in OpenFoam. The solver includes two main equations solved sequentially: the continuity equation accounting for the pyrolysis gas production (source term) and the energy conservation (including heat transfer, gas convection, and the enthalpy change of the solid and of the gases). This module has been used to compute the case presented in Fig. 1.

1- Introduce the momentum conservation in porous media (Darcy's law). The second module, PAT-1, is intended to analyze 3D gas convection effects on the temperature gradient in the material. We are currently re-analyzing Stardust re-entry using this model.

2- Chemical evolution of the pyrolysis gases in the material: finite-rate pyrolysis of the pyrolysis gases, reaction of the pyrolysis gases with the air diffusing inside the material. The chemistry class of OpenFoam is included in PAT-1. In order to independently refine the chemistry model, the `reactingFoam` solver has been simplified into a 0D solver.

OpenFoam can conveniently be used *in lieu* of a chemistry solver. We present in Fig. 3 the evolution of the pyrolysis gas composition at 1500K according to an improved version of the chemistry model of April [11].

4- Modeling of TPS with holes (pressure-sensor passages for example). This is part of the objectives of the capability development effort. We plan to use the Darcy-Brinkman model for transport in porous media. The porous medium class of OpenFoam will be used for this solver. We plan to turn the steady-state solver available into a time accurate solver.

5- New description of ablation as a volume phenomenon (the material mass may be depleted in depth): a porous medium approach will be used following the guidelines given in ref. [5]. For this future work, we plan to use a volume of fluid approach instead of a moving mesh.

We are currently considering extending the presented plan to include flow-material coupling. Our starting point would be to link the hypersonic chemistry library of Prof. Thierry Magin (at the von Karman Institute) to OpenFoam.

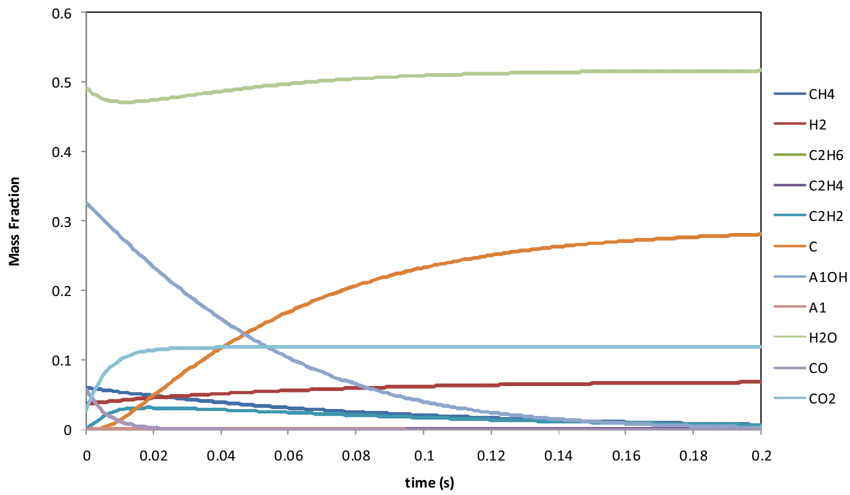


Fig. 3 - Evolution of the pyrolysis-gas composition at 1500K. The equilibrium composition is reached after 0.2 s.

(1) Stardust is an interplanetary mission, whose primary purpose was to collect cosmic dust from the comet Wild 2 and to return it to Earth. Stardust re-entered the Earth atmosphere at a record velocity of 12.7 km/s in January 208.

Key words: Atmospheric re-entry, Ablation, Pyrolysis, Heat and mass transfer, Finite-rate chemistry, Front tracking

References

[1] Stackpoole, M., Sepka, S., Cozmuta, I., and Kontinos, D., "Post-Flight Evaluation of Stardust Sample Return Capsule Forebody Heatshield Material," AIAA paper 2008-1202, Jan. 2008.
[2] Tran, H. K., Johnson, C. E., Rasky, D. J., Hui, F. C. L., Hsu, M.-T., Chen, T., Chen, Y. K., Paragas, D., and Kobayashi, L., "Phenolic Impregnated Carbon Ablators (PICA) as Thermal Protection Systems for Discovery Missions", NASA Technical Memorandum 110440, 1997.
[3] http://www.spacex.com/press.php?page=20090223
[4] Ritter, H., Portela, P., Keller, K., Bouilly, J. M., and Burnage, S., "Development of a European ablative material for heatshields of sample return missions," 6th European Workshop on TPS, Stuttgart, Germany, 1-3 April 2009.
[5] Lachaud, J., Cozmuta, I., Mansour, N. N., "Multiscale Approach to Ablation Modeling of Phenolic Impregnated Carbon Ablators", Journal of Spacecrafts and Rockets, under press. Preprint online: www.jeanlachaud.com/research
[6] S. Sepka and M. Wright, A Monte Carlo Approach to Fiat Uncertainties - Improvements and Results for MSL, AIAA-2009-4234.
[7] Moyer, C. B., and Rindal, R. A., "An analysis of the coupled chemically reacting boundary layer and the charring ablator", NASA CR-1061, 1968.
[8] Milos, F. and Chen, Y.-K., "Ablation and Thermal Response Property Model Validation for Phenolic Impregnated Carbon Ablator," AIAA paper 2009-262, Jan. 2009.
Two-Dimensional Ablation and Thermal Response Analyses for Mars Science Laboratory Heatshield
[9] Chen, Y. -K., Gokcen, T., Edquist, K., "Two-Dimensional Ablation and Thermal Response Analyses for Mars Science Laboratory Heatshield", AIAA paper 2009-4235, June 2009.
[10] Beerman, A., Lewis, M., Starkey, R., and Cybyk, B., "Nonequilibrium Surface Interactions Ablation Modeling with the Fully Implicit Ablation and Thermal Response Program," AIAA paper 2008-1224, Jan. 2008.
[11] April, G. C., "Energy Transfer in the char Zone of a Charring Ablator", Ph. D. Dissertation, Department of Chemical engineering, Louisiana State University, 1969.