Modeling and simulation of chemical reactions at the surface of an ablative wall interacting with a hypersonic flow: Application to atmospheric reentry

Guillaume Coria*
French Air Force Academy, Salon Air, 13661, France

Dr Jean-Denis Parisse†
French Air Force Academy, Salon Air, 13661, France

Dr Jean-Michel Lamet‡ & Dr Nicolas Dellinger§
French Aerospace Lab ONERA, Toulouse, 31000, France

The present work is devoted to the modeling and simulation of the degradation of ablative carbon composite materials used as Thermal Protection System (TPS) for hypersonic reentry vehicles. Detailed models of oxidation, nitridation and sublimation are implemented in the 3D finite volume material response code MoDeTheC. In order to simulate thermal degradation and surface regression of the TPS, the strategy is based onto a coupling between MoDeTheC and the CEDRE Computationnal Fluid Dynamic (CFD) code, both developed by ONERA.

Firstly, reaction mechanisms from the literature are compared on an elementary test case. Secondly, the degradation models and the coupling strategy between MoDeTheC and CEDRE are applied to the simulation of a flight point on the trajectory of the experimental flight RAM-C I for which reference data are available in the literature.

Keywords :
Ablation, atmospheric entry, oxidation, nitridation, sublimation.

I. Introduction

The atmospheric reentry of space objects is the place of many physical phenomena which immerse them to extreme conditions. The strong detached shock created ahead space objects transmits very large heat fluxes to the TPS. The huge energy to be dissipated (of the order of a mega-joules) requires the use of TPS made of ablative materials (generally carbon-based composites) to ensure the survival of the objects' structure. The multi-physical character and the extreme conditions intrinsic to ablation make it difficult to experiment those phenomena in the laboratory. Even today, TPS design is based on important safety factors. Numerical simulation appears to be an essential tool for reducing these safety margin, and, among others, the weight in the TPS design. This paper is part of this process of improving computational tools related to ablation degradation. After a description of the chosen chemical models, the models implemented in the MoDeTheC solver, developed at ONERA to simulate the thermal degradation of composite materials, are validated on a simple test case. Finally, the MoDeTheC code, coupled with the CEDRE CFD code, is confronted to reference data available in the literature for the experimental flight RAM-C I carried out by National Aeronautics and Space Administration (NASA)[1, 2].

II. Chemical models and methods

First of all, surface oxidation (respectively nitridation) is the reaction between an atom or molecule containing oxygen (respectively nitrogen) and the TPS, or more specifically, the carbon atoms of the wall surface. Sublimation is a phase change from the solid state directly to the gaseous state. In the present study, oxidation and nitridation are encountered above 800K while sublimation occurs above 2500K[3–5]. Those chemical reactions, which participate in

*PhD student, Centre de Recherche de l'école de l'air, guillaume.coria@ecole-air.fr, AIAA student member.
†Associate Professor, Centre de Recherche de l'école de l'Air, jean-denis.parisse@ecole-air.fr.
‡Research engineer, Multi-physics department for energy, jean-michel.lamet@onera.fr.
§Research engineer, Multi-physics department for energy, nicolas.dellinger@onera.fr.

the regression of the wall, consume the chemical species present in the flow and produce carbonated gaseous species while ablating the wall.

A. Chemical models

Two models were selected to be implemented in MoDeTheC, namely the models of Duffa [3] and Zhluktov & Abe[4]. From temperature, pressure and chemical composition conditions at the wall surface, they both provide the surface mass flow rate of carbon ($kg.m^{-2}.s^{-1}$) from which the regression speed of the wall ($m.s^{-1}$) is deduced. They also allow computing of the surface mass flow rates of involved gaseous species consumed and produced at the wall.

Duffa's model[3] Duffa describes oxidation, nitridation an sublimation with reversible chemical reactions. He also introduces the concept of an active site, which corresponds to an available bond of a carbon atom at the wall surface where an oxigen or nitrogen atom can be stuck. The surface reaction mechanism is based on the models of Eley-Rideal and Langmuir-Hinshelwood. Moreover, this model use Arrhenius' laws to determine the kinetic constants of each reactions.

Zhluktov & Abe's model[4] The model of Zhluktov & Abe improves Duffa's one. The model for calculating the kinetic constants of each reaction is more exhaustive and takes into account the dissociation of the molecules of the environment.

B. Methods

Firstly, the chemical kinetic reactions models implemented in MoDeTheC are compared on a simple test case without coupling with the hypersonic flow response. The produced gases are therefore not taken into account and a stationary regime is assumed.

Secondly, the study focuses on the simulation of the flight point at 40km (Mach 23.3) extracted from the trajectory of the RAM-C I space probe [1, 2], for which comparative data are available in the literature. The hypersonic flow arround the RAM-C I probe is simulated with the CEDRE code and the degradation of the probe's ablative wall (made of phenolic carbon NARMCO 4028[1]) with the MoDeTheC code. In addition to a classical heat flux - temperature coupling, both codes are coupled at the fluid/solid interface in order to compute the species source terms and the interface regression speed from the gas pressure and composition.

III. Preliminary results

The surface regression speed, calculated by taking into account only oxidation, is presented in figure 1 as a function of the wall temperature and gas pressure at the wall. The environment is here assumed to be composed of air at equilibrium for each temperature. The overall behavior of the models in temperature and pressure evolution are similar. Indeed, at low temperature, the regression rate is close to zero. Then, for a temperature close to 1000K, the chemical reactions are activated and increase the regression speed. For temperatures above 1800K, the regression speed keeps increasing exponentially with temperature. This phenomenon due to oxidation is not observed in reality, since the regression speed should reach a plateau. This is explained by the fact that from those temperatures, the kinetics of oxidation reactions are controlled by the diffusion of species through the boundary layer. However, both models do not account for this control by diffusion, since the composition of the gas at the wall being imposed with no feedback from the gases (CO and CO_2) produced or consumed at the wall.

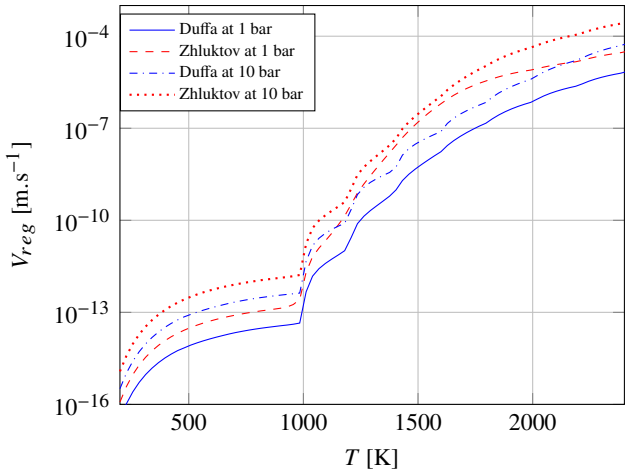

Fig. 1 Regression speed due to oxidation - non-coupled results

The oxidation model is applied to the simulation of the flight point at 40km of the RAM-C I mission. Figure 2 shows the regression of the wall (initially placed at X = 0 m) after 5s. On the fluid side, the gas composition in the boundary layer is clearly affected by the recession, locally and also along the probe due to advection. In particular, the mass fraction of atomic oxigen decreases and the one of CO and CO_2 increases, as expected. This allows verifying the behaviour of the oxidation model and of the coupling procedure between the material and the fluid.

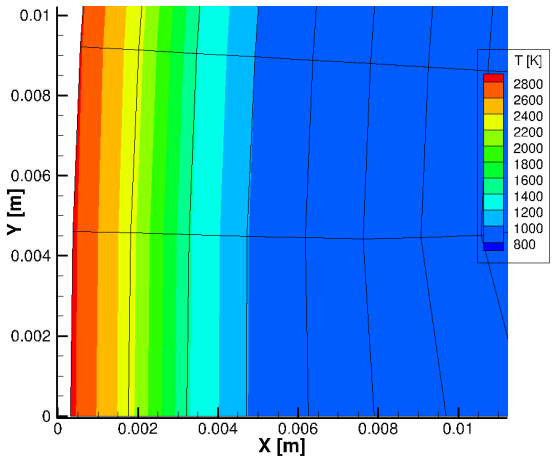

Fig. 2 Solid mesh regression due to Duffa's oxidation model and temperature diffusion for RAM-C I flight simulation (altitude = 40km and simulation time = 5s)

Results of final manuscript : The final manuscript will include the results obtained with the complete chemical models on both the simple test case and a trajectory point of the RAM-C I mission. The numerical results on the RAM-C I probe will be compared to reference data available in the literature.

IV. Conclusion

The interaction between a hypersonic flow and an ablative wall during an atmospheric reentry is complex to model because of the diversity of physical phenomena involved. Among those multi-physical phenomena, this work improve the numerical modeling of surface chemical reactions by implementing detailed reactions models. Two models have, therefore, been implemented in the material code MoDeTheC. They were confronted to reference data from the literature on the RAM-C I flight at the altitude of 40km by coupling MoDeTheC with the CFD code CEDRE.

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