Computational Analysis of Hypersonic Flows Including Finite Rate Ablation Thermochemistry

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INTRODUCTION

The main objective of the present activity is to improve the computational fluid dynamics (CFD) capabilities and the simulation and understanding of the complex physico-chemical mechanisms (such as oxidation, sublimation and pyrolysis gas injection) which are involved at the interface between thermal protection system (TPS) materials and the aerodynamic flowfield in reentry conditions. The practical interest in the thorough understanding and control of these surface phenomena is associated to their impact on the design and sizing of the TPS. This problem is of critical importance for optimization of the TPS for future hypersonic vehicles and spacecraft. In fact, heatshields for atmospheric reentry vehicles are being designed at present mostly using computer codes because ground test facilities, though extremely helpful, cannot adequately replicate flight conditions. Thermal protection systems are traditionally designed with one and two-dimensional engineering codes. Occasionally, a detailed CFD computational solution is obtained, but these solutions rarely contain the correct boundary conditions. In fact, CFD codes typically treat fluid/solid surface boundary conditions in a very simplified or idealized manner such as a constant prescribed temperature or heat flux and with zero mass transfer. However, in energetic hypersonic environments, TPS materials interact with the flow through diverse thermochemical and thermophysical mechanisms including ablation, shape change, pyrolysis, melt flow, and spallation. Even in the nonablating case, real materials conduct heat, catalyze reactions, and participate in radiative energy exchange. However, most codes use primitive surface boundary conditions and cannot realistically be used for TPS design. CFD calculations rarely take into account spatially varying surface temperature and heat flux, a realistic surface energy balance (accounting for ablation, pyrolysis and surface chemical reactions), thermal soak into the TPS material, and thermochemical ablation modeling. To compensate for uncertainties in the analyses, a safety margin of extra TPS material is added to the final design, and the structural weight must also be increased. Clearly there is a need for more accurate, multidimensional computational tools which can be used to reduce the uncertainties in TPS analysis and to optimize the TPS distribution around hypersonic vehicles and spacecraft. The major goal of this research project is the improvement of the numerical modeling capabilities through the development of advanced CFD tools with gas-surface interaction capabilities. The main objective is to reduce empiricism, and to increase fundamental modeling capability through increased understanding.

NUMERICAL METHOD AND APPROACH

The CFD code used in this activity is a finite-volume solver for three-dimensional compressible flows developed in-house. The code, which adopts a standard finite volume Godunov-type formulation, is second order accurate in both space and time and uses multi-block structured meshes. The system of equations is approximated by a cell-centered finite volume scheme. The viscous fluxes are approximated by centered differencing, whereas the convective fluxes are computed by means of the solution of a Riemann problem whose left and right states are reconstructed by an interpolation procedure which uses the min-mod limiter. The system of ordinary differential equations is advanced in time by means of an explicit Runge-Kutta integration. In addition, the code has been parallelized using the OpenMP directives and it can run on SMP computers.

In this work, the formulation of finite rate ablation surface boundary conditions, including recombination, oxidation, nitridation, and sublimation of carbonaceous materials with pyrolysis gas, is developed and integrated with a 3-D Navier Stokes solver. The kinetic model adopted for gas/surface interactions is based on the work of Park [1, 2, 3]. These boundary conditions, based on species mass conservation and steady state surface energy balance, are discretized and integrated with the CFD code to predict the aerothermal heating, the surface temperature, the gas-phase chemical species concentrations, and the carbon ablation rate. The concentrations of all surface chemical species will be determined from gas-surface chemical reactions balanced by mass transfer rate. The surface temperature and heat flux will be determined from the surface energy balance where the conduction flux into the solid will be computed assuming steady-state ablation. The surface recession rate and the surface temperature are thus obtained as part of the flowfield solution. This will permit to bypass all of the classical approximations such as equilibrium thermochemical tables, heat and mass transfer coefficients, and blowing correction approximations which needs to be used when ablating boundary conditions are not accounted for in the CFD solution. The mass and energy surface balances, combined with suitable ablation models, provide complete surface thermochemistry conditions for the multidisciplinary numerical solution of the coupled CFD/ablation problem for TPS analysis. The computation model developed in this work will be used to simulate carbonaceous material (such as graphite and carbon-phenolic) ablation during Earth reentry.

RESULTS

The modeling of gas/surface interactions has been the subject of considerable interest recently, because the coupling that occurs has been shown to have a dramatic effect on the net heating level induced by the gas and on the response of the heat-shield surface [4, 5, 6]. In most fluid-solid coupling computations, the ablative carbon surface is assumed to be at chemical equilibrium. Chemical equilibrium is a good assumption for many space entry applications, but may not be valid for all conditions [7, 8]. Moreover, when non-ablating CFD calculations are performed, an engineering correlation with blowing reduction parameter has to be introduced in the simulation to take into account the effect of mass injection on reduction of convective heat flux. A mass transfer coefficient also has to be defined based on the heat transfer coefficient under the assumption of thin boundary-layer for the computation of the char recession rate. The purpose of this work is to present a tightly coupling of a detailed finite-rate gas/surface reaction model to a three-dimensional chemically-reacting fluid dynamics (CFD) code.

The presented test case is a study of the interaction between a graphite model and an arc-jet stream, conducted in the Interaction Heating Facility (IHF) at the NASA Ames Research Center. The stream total enthalpy is estimated to be about 27 MJ/kg, and the measured stagnation point pressure is 0.8 atm. Other calculated freestream quantities are listed in Table 1. In this arc stream, oxygen is fully dissociated and nitrogen is partially dissociated. The graphite model is a 10 half angle sphere-cone with nose radius of 1.905 cm. The total length of the model is 8.89 cm. Surface temperature distribution was measured

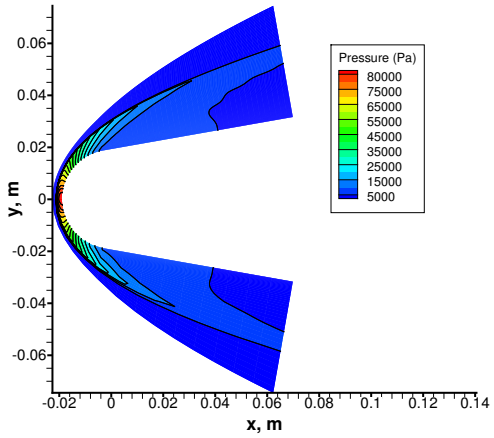
Table 1: Freestream condition for graphite test case

Property	Value
Velocity	5354 [m/s]
Density	0.003 [kg/m^3]
Temperature	1428 [K]
Mass concentrations	
y_{O_2}	0.0001
y_{N_2}	0.6169
y_{NO}	0.0046
y_N	0.1212
y_O	0.2572

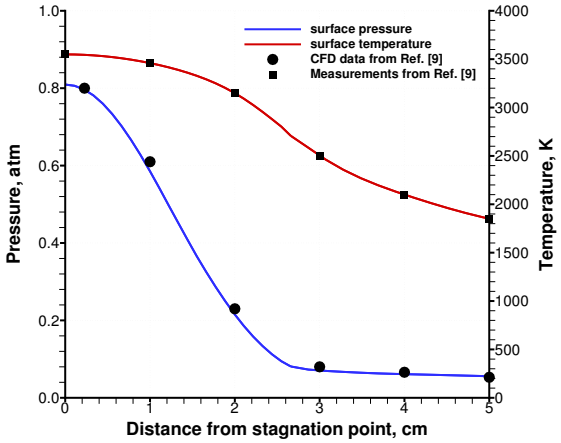
using an infrared camera and pyrometers. Therefore, in the numerical rebuilding, the surface temperature profile is specified at the surface based on the measurement.

Two-dimensional axisymmetric simulations have been performed to numerically reproduce this test case. A single-block grid composed of 30×80 grid points in the axial and normal directions, respectively, is adopted. The grid is constructed such to ensure orthogonality at the surface and is adapted to the Mach contours to achieve proper grid alignment to the shock. In the normal direction, meshes are clustered near the body surface such to accurately capture the near wall phenomena. A grid convergence analysis is also performed to ensure that results are grid independent, performing simulations on a coarse 15×40 and a fine 60×160 grid. All the computations presented are at steady-state condition. The ablation species considered are CO (oxidation), CN (nitridation) and C_3 (sublimation) while the air species are those listed in Table 1. The overall number of species included in the gas is 11, including the species originating from gas-phase dissociation and exchange reactions of the ablation species producing C, C_2, and CO_2. The wall boundary condition includes finite-rate ablation and blowing. The gas-phase chemical reactions implemented in the CFD code are taken from the work of Olynick et at. [9] for Stardust earth entry simulation and are mainly derived from the work of Park [3, 10].

Flowfield pressure contours are reported in Figs. 1(a) showing the bow shock ahead of the body. The predicted stagnation point pressure is 0.81 atm in good agreement with the experimental data of 0.80 atm reported in Ref. [7]. The surface temperature and pressure profiles are shown in Fig. 1(b). Surface temperature distribution was measured using an infrared camera and pyrometers. Thus, instead of solving the steady-state energy balance, the surface temperature profile is specified based on the measurement. Figure 1(b) has been obtained assuming a fully reactive flowfield and ablative wall, however, the surface pressure profile is essentially unaffected by the gas-phase and surface chemistry conditions. Predicted carbon mass blowing rate distributions over the model surface are shown in Fig. 2(a). The green line is the prediction based on the Park's surface kinetics with the nitridation surface reaction and the red line is without the nitridation reaction. Surface recession data are measured at stagnation point and at 45-deg from the stagnation point. The symbols in Fig. 2(a) are the mean graphite mass blowing rates of a 30 sec heat pulse. Without the nitridation reaction, the finite-rate model slightly overpredicts the mass blowing rate by about 4% at the stagnation point, and underpredicts it by about 10% at 45 deg from the stagnation point. Including the nitridation reaction, the difference between prediction and measurements is about 43% at the stagnation point and is about 37% at 45 deg from the stagnation point. Clearly, the inclusion of the nitridation reaction in Park's surface kinetics tends to overpredict the experimental data. Figure 2(b) shows the chemical species distributions along the stagnation streamline for Park's finite rate

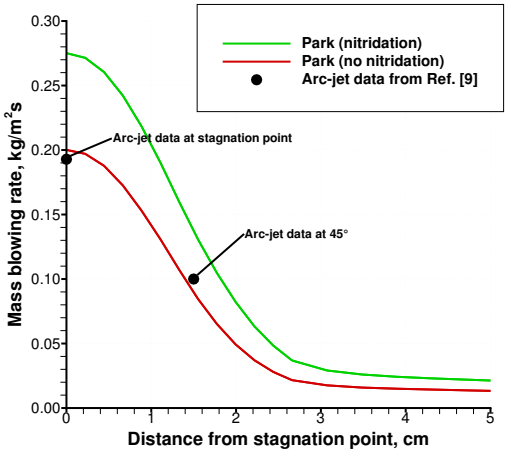


(a) Pressure contours in the flowfield. Comparison of the coarse (bottom) and fine grid (top).

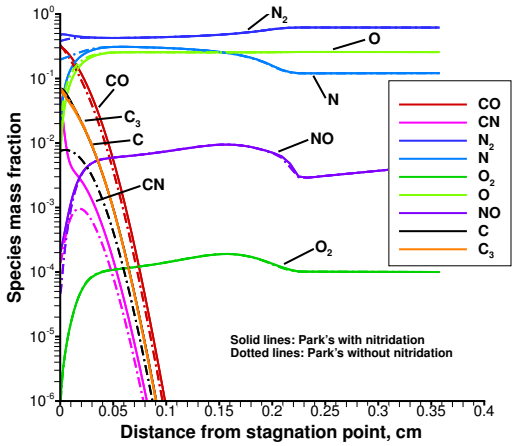


(b) Surface temperature (imposed from measurements) and pressure distributions along graphite surface.

Figure 1: Pressure contours and surface profiles.



(a) Measured and predicted carbon mass blowing rate distributions for various surface chemistry conditions.



(b) Chemical species distributions along the stagnation streamline with and without surface nitridation (minor species including CO_2 and C_2 have not been plotted for clarity).

Figure 2: Ablation mass rate and chemical species distributions.

model with and without nitridation using the 17-reaction finite-rate chemistry model. The major ablation products present at the surface are CO, C_3, and CN from carbon oxidation, sublimation, and nitridation, respectively. Both atomic and molecular oxygen are consumed at the surface by the oxidation reactions, although the molecular oxygen mass fraction is so small that its contribution to carbon oxidation is negligible. Molecular nitrogen is further dissociated in the shock layer. When surface nitridation is activated, atomic nitrogen is fully consumed at the surface. The effect of considering or neglecting the nitridation reaction is clearly affecting the solution close to the surface.

In the final work other test cases will be presented, including different ablative materials such as carbon-phenolic, to show also the effect of pyrolysis gas injection. Moreover, a systematic parametric analysis will be performed to study how the prediction of surface recession and convective heat flux is sensitive to the surface kinetic model and the gas-phase reaction model.

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