Sensitivity Analysis of the Gupta and Park Chemical Models on the Heat Flux by DSMC and CFD Codes

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Abstract. The present study is the logical continuation of a former paper by the first author in which the influence of the chemical models by Gupta and by Park on the computation of heat flux on the Orion and EXPERT capsules was evaluated. Tests were carried out by the direct simulation Monte Carlo code DS2V and by the computational fluid-dynamic (CFD) code H3NS. DS2V implements the Gupta model, while H3NS implements the Park model. In order to compare the effects of the chemical models, the Park model was implemented also in DS2V. The results showed that DS2V and H3NS compute a different composition both in the flow field and on the surface, even using the same chemical model (Park). Furthermore DS2V computes, by the two chemical models, different compositions in the flow field but the same composition on the surface, therefore the same heat flux. In the present study, in order to evaluate the influence of these chemical models also in a CFD code, the Gupta and the Park models have been implemented in FLUENT. Tests by DS2V and by FLUENT, have been carried out for the EXPERT capsule at the altitude of 70 km and with velocity of 5000 m/s. The capsule experiences a hypersonic, continuum low density regime. Due to the energy level of the flow, the vibration equation, lacking in the original version of FLUENT, has been implemented. The results of the heat flux computation verify that FLUENT is quite sensitive to the Gupta and to the Park chemical models. In fact, at the stagnation point, the percentage difference between the models is about 13%. On the opposite the DS2V results by the two models are practically equivalent.

Keywords: Heat Flux, EXPERT capsule, DSMC, CFD
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INTRODUCTION

It is well known that one of the most important problems in the design of a capsule is the evaluation of heat flux during the re-entry. This evaluation has to provide information about the design of the Thermal Protection System (TPS). Such an analysis should be carried on experimentally in thermal tunnels but, as well known, studying experimentally any aerodynamic problem in hypersonic, rarefied flow is very difficult and expensive. For this reason, computational methods play an important role and are subjected to continuous improvements. In this specific topic, the chemical model is crucial because it influences the gas composition in the flow and then, due to the exo/endothermic characteristic of the reactions, also the heat flux.

In a former paper by Morsa et al. [1], the comparison of the heat flux computations in high altitude flight, by two codes based on different philosophies, was carried out. A code solves the flow field by the direct simulation of the molecules evolution (direct simulation Monte Carlo method: DSMC), the other one relies on the solution of the Navier-Stokes equation (computational fluid dynamics: CFD). The DSMC code was DS2V [2], the CFD code was H3NS [3]. DS2V implements the Gupta chemical model [4], while H3NS implements the Park chemical model [5], [6] and [7]. The results showed that the heat flux by DS2V was always higher that the one by H3NS. The reason was that the two codes compute different chemical compositions. Therefore, a sensitivity analysis of the chemical models was carried out. More specifically, the Park model was implemented also in DS2V and the related results were compared with those by the Gupta model. Tests were carried out for the EXPERT and Orion capsules in the high altitude path of the re-entry trajectories. The results showed for both capsules that DS2V and H3NS computed a different chemical composition both in the flow field and on the surface, even using the same chemical model (Park). For this reason, the difference in the computation of heat flux between DS2V and H3NS was attributed mostly to the different handling of the chemical process.

In the present work, in order to evaluate the influence of the chemical models also in a CFD code, the Gupta and the Park models have been implemented in the well known and widely accepted CFD code FLUENT [8]. Tests were carried out for the EXPERT capsule at an altitude of 70 km and with velocity of 5000 m/s. At this velocity, the specific kinetic energy (1.25×10^6 J/kg) is high enough to activate the molecule vibration degree of freedom (for

Oxygen 5.92×10^5 J/kg, for Nitrogen 9.99×10^6 J/kg) but is not high enough to activate ionization (the minimum ionization energy is for nitric oxide 2.98×10^7 J/kg). For these reasons, the vibration equation, lacking in the original version of FLUENT, has been implemented; as well as the chemical model have been implemented with no ionization reactions; air is considered as made up of five, neutral chemical species: O_2, N_2, O, N and NO.

THE GUPTA AND THE PARK CHEMICAL MODELS

The five neutral chemical species (O_2, N_2, O, N, NO) react according to 17 forward/backward chemical reactions by the Gupta and the Park models. In the Gupta model, both the forward (k_f) and the backward (k_b) rate coefficients are expressed in terms of the Arrhenius-like equation:

$$k_{f,b} = C_{f,b} T^{n_{f,b}} \, exp\left(- \frac{E_{a_{f,b}}}{kT} \right). \tag{1}$$

where C is the pre-exponential factor, n is the temperature exponent, E_a is the specific activation energy, k is the Boltzmann constant, subscripts f and b stand for forward and backward reactions. Park provides the forward reaction rate coefficients expressed in the Arrhenius-like equation:

$$k_f = C_f T^{n_f} \, exp\left(- \frac{E_{a_f}}{kT_c} \right). \tag{2}$$

where T_c is the temperature controlling the reaction. This temperature takes into account the influence of the vibrational temperature on the rates of reaction. Park assumes that T_c is a function of the geometrical mean temperature between the transitional and the vibrational temperatures:

$$T_c = T^{\phi} T_v^{(1-\phi)}. \tag{3}$$

where, according to Park [6], ϕ=0.5 for dissociation/recombination reactions and ϕ=1.0 for exchange reactions. The backward rate coefficient (k_b) is computed by the ratio of the forward rate coefficient (k_f) and the equilibrium constant (K_e): $k_b=k_f/K_e$.

For a direct comparison of the Gupta and of the Park models, Figs.4(a) thru (f) show the profiles of forward and backward reaction rates for some reactions as a function of temperature in the interval 3000-13000 K. These reactions have been chosen because are the most frequent in the present application. Figures show that: i) the reaction rate coefficients are comparable, ii) neither the Gupta model nor the Park model is always prevalent on the other one.

Handling the chemical processes in DSMC is different from that in CFD. In fact a DSMC code does not rely on the rate equation (Eqs.1, 2) but uses only the pre-exponential factor ($C_{f,b}$), the temperature exponent ($n_{f,b}$) and the activation energy ($E_{af,b}$) to calculate the reaction probability (or steric factor [9]). For this reason, in order to implement the backward reaction rates of the Park model in DS2V or to define C_b, n_b and E_{ab}, the curves best-fitting the values k_f/K_e as a function of temperature, were obtained in the form of Eq.1 [1].

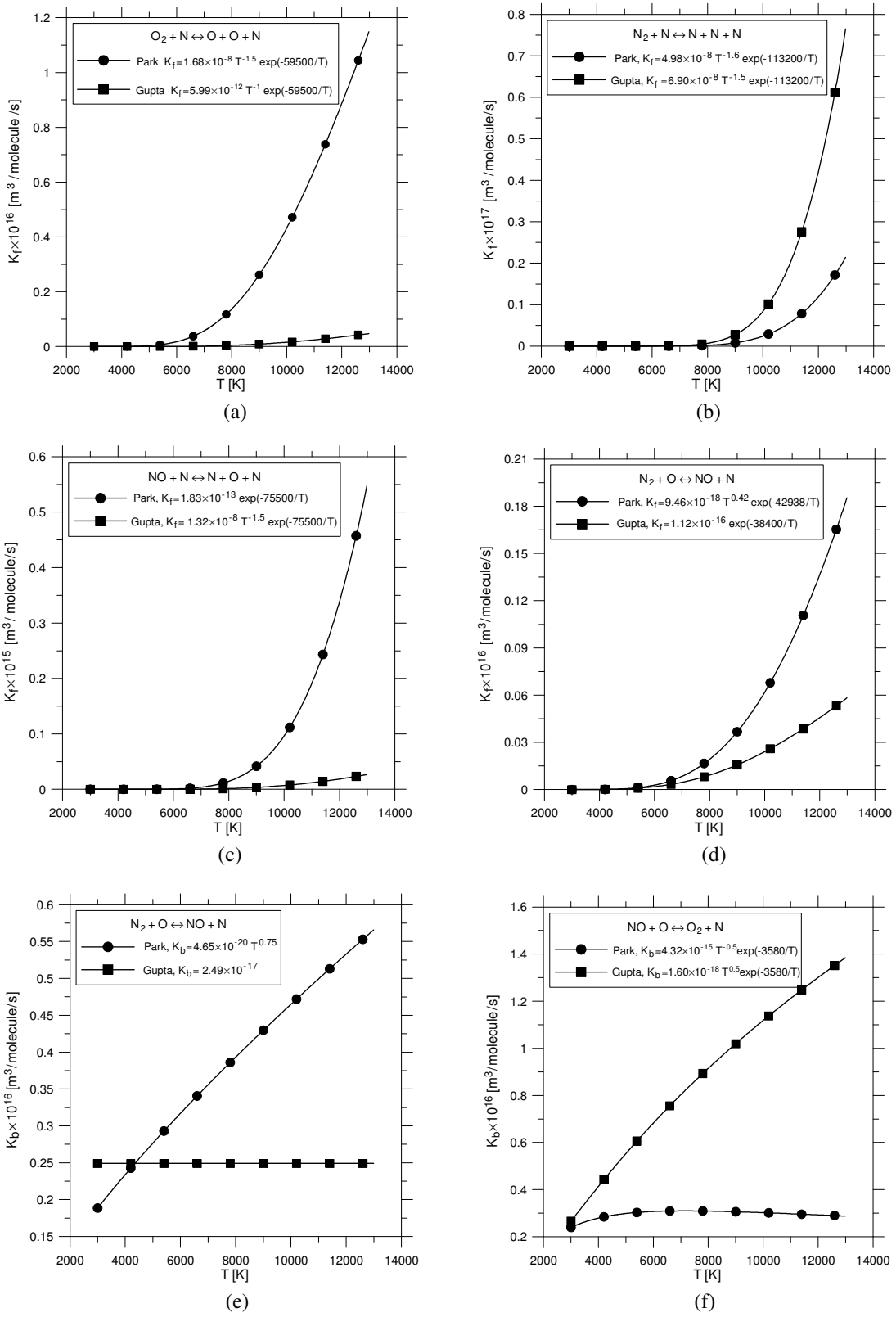

FIGURE 1. Profiles of the forward (a,b,c,d) and backward (e,f) reaction rates of some reactions by the Gupta and the Park models

EXPERT CAPSULE

The ESA capsule EXPERT (European eXPErimental Reentry Testbed) was designed to enhance knowledge of aero-thermo-dynamic problems during the re-entry. The capsule will be transported by a Russian VOLNA rocket at an altitude of about 105 km and then released; it will follow a ballistic re-entry trajectory. Figure 2 shows the current baseline geometries of EXPERT; it is a blunted pyramidal shape, consisting of a body of revolution with an ellipse-clothoid-cone 2D longitudinal profile. The angle of the cone is 12.5 deg., the total length is 1.55 m and the base diameter is 0.918 m. The longitudinal profile is cut by 4 planes at an angle of 8.35 deg. to the axis of symmetry. Each plane is equipped with an open flap. Each flap, width 0.4 m and length 0.32 m, is deflected by 20 deg. with respect to the related plane. The nose, or the fore part up to x=0.40 m, has a local radius of 0.6 m at the stagnation point, a base diameters (D) of 0.36 m and an eccentricity of 2.5.

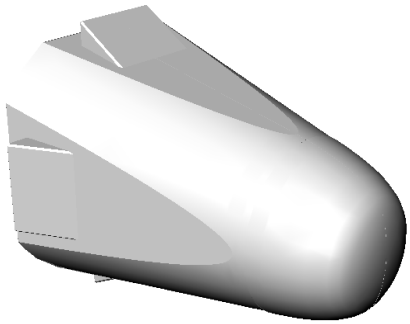

FIGURE 2. EXPERT capsule

COMPUTING CODES

Due to the cut planes and flaps, EXPERT is not axial-symmetric, but the nose is an axial-symmetric body. Considering that the tests have been carried out at zero angle of attack (α), it has been possible to simulate only this part of EXPERT by the 2-D DSMC code DS2V and by FLUENT, running in 2-D/axial-symmetric mode.

DS2V is able to consider air as a built-in gas. Air is considered made up of five chemical species (O_2, N_2, O, N, NO) in thermo-chemical non equilibrium. The built-in chemical model is the Gupta model. The code is "sophisticated" and advanced. DS2V is "sophisticated" (a sophisticated code is termed also DSMC07) [10] thru [13] and advanced. A DSMC07 code relies on the same theoretical basis like an original DSMC code (termed also DSMC94), but implements computing procedures making it far more efficient and more accurate than a DSMC94 code. Besides being sophisticated, DS2V is also advanced, allowing the user to evaluate the quality of a run in terms of the adequacy of the number of simulated molecules by the "on line", i.e. during the run, visualization of the ratio of the molecule mean collision separation (mcs) and the mean free path (λ) in the same cell; mcs/λ should be less than unity everywhere in the computational domain. Bird [2] suggests 0.2 as a limit value for an optimal quality of the run.

The CFD code FLUENT solves the governing equations of continuity, momentum, energy and species transport simultaneously as a set, or vector, of equations and uses a control-volume-based technique to convert a general scalar transport equation to an algebraic equation that can be solved numerically. This control volume technique consists in integrating the transport equation about each control volume, yielding a discrete equation that expresses the conservation law on a control-volume basis. Turbulence and governing equations for additional scalars (UDS) (as per vibrational energy) can be solved sequentially. With such UDSs, the FLUENT core manages vibrational relaxation, chemical reaction, species properties and wall boundary conditions, etc.. Vibration equation, implemented in this application, reads:

$$\frac{\partial(\rho e_{vj})}{\partial t} + \underline{\nabla} \cdot (\rho \underline{V} e_{vj}) = \dot{e}_{vj}. \tag{4}$$

Vibrational relaxation is modeled by the Landau-Teller [14[, [15] formulation. Relaxation time is obtained by Millikan and White [16], assuming simple harmonic oscillators. Furthermore, in order to take into account the turbulence effects, the Spalart-Allmaras model [17] is used. This model solves a modeled transport equation for the kinematic turbulent viscosity.

ANALYSIS OF THE RESULTS

Test conditions are those met by EXPERT at the altitude of 70 km and with velocity of 5000 m/s. At this altitude the capsule experiences a hypersonic continuum low density regime; the Mach number is 17 and the Knudsen number, based on the nose diameter is $Kn_{D\infty}=2.77\times10^{-3}$. According to Moss [18], a general definition of the transitional regime is: $10^{-3}<Kn_{D\infty}<50$.

Figures 3(a) and (b) show the profiles of atomic Oxygen and atomic Nitrogen along the stagnation line of EXPERT predicted by FLUENT and by DS2V, both using the Gupta and the Park chemical models. FLUENT and DS2V are in agreement in calculating, in the flow field, a molar fraction of atomic species by the Park model higher than the ones by the Gupta model. Therefore, the Park model is more reactive than the Gupta model. However FLUENT keeps the difference between the models also toward the surface, on the opposite DS2V tends to reduce this difference. This can be also verified by the molar fractions of air at the stagnation point reported in Table 1. The molar fractions, computed by the two models, are not very different for DS2V, while they are pretty different for FLUENT. As already shown in Figs. 1(a) to (f), the difference of the rate coefficients by both models tend to reduce with decreasing temperature. Considering that toward the surface the flow field temperature decreases, DS2V appears to meet expectations better than FLUENT.

Figure 4 shows the profiles of temperature along the stagnation line by the two codes for both chemical models. As expected, due to the higher reactivity of the Park model, temperature by Park, computed by both codes, is lower than the one by Gupta. More specifically, the maximum values of temperature by DS2V are 13230 K for Gupta and 11849 K for Park, those by FLUENT are 9450 for Gupta and 9100 for Park.

The influence of the two chemical models produces slight variation in the stand-off distances of the shock waves. In fact, the differences are only about 0.0025 m for DS2V and 0.0019 m for FLUENT. Even though these variations are very small indeed, however they produce locally strong effects. For instance, at position $x\cong-0.043$ m, temperatures by Gupta and by Park in the DS2V code are about 13000 K and 2800 K, in FLUENT at position -0.041 m are about 1000 K and 9000 K.

Figure 5 shows the profiles of heat flux along the nose surface. Considering that DS2V predicts practically the same composition on the surface, it also computes practically the same heat flux. On the opposite, the different composition computed by FLUENT influences the heat flux computation. The heat flux at the stagnation point computed by the Gupta model is about 13% higher than the one computed by the Park model. This is due, as already said, to a lower reactivity (dissociation) of the Gupta model; this means that a lower amount of energy is spent for dissociation and then a higher amount of energy is exchanged with the surface. The lower values of heat flux, predicted by FLUENT using both chemical models, compared with those predicted by DS2V, is justified by an higher reactivity of FLUENT than the one of DS2V. In fact, as reported in Table 1, the values of molar fraction of atomic species, computed by FLUENT, are higher than the ones predicted by DS2V. For completeness, the heat flux profile by H3NS, implementing the Park model, is also shown in the same figure. As expected, this profile is in good agreement with the one predicted by FLUENT.

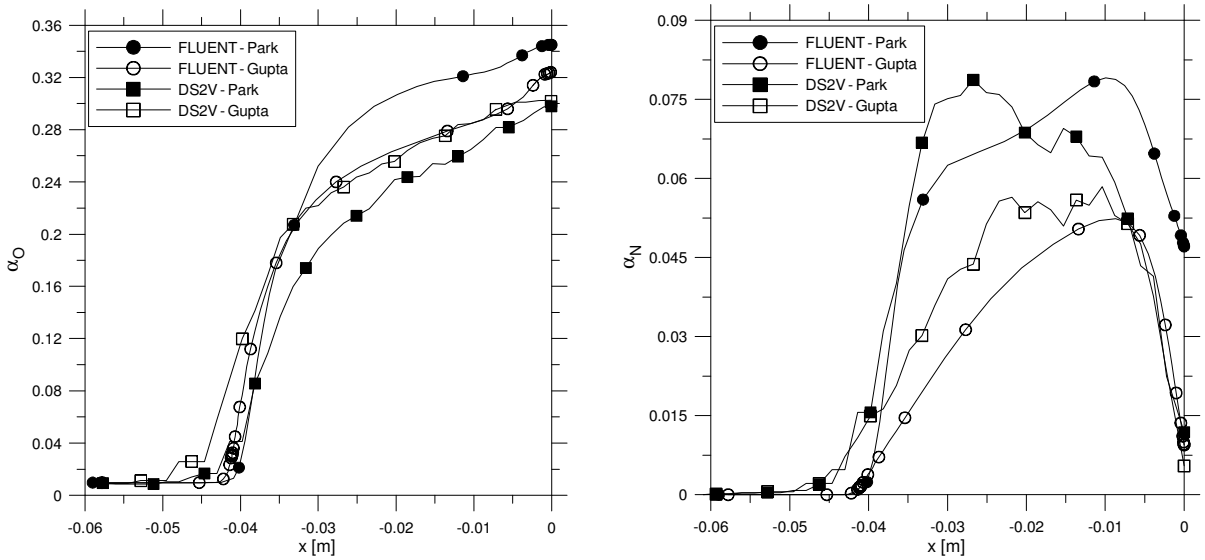

FIGURE 3. Molar fraction of O (a) and N (b) along the stagnation line of EXPERT computed by FLUENT and by DS2V: non reactive surface, h=70 km

TABLE 1. Molar fractions at the stagnation point of EXPERT: h=69.8 km, non-reactive surface

Code - Chemical Model	α_{O_2}	α_{N_2}	α_O	α_N	α_{NO}
FLUENT - Gupta	0.00525	0.645	0.3253	0.00943	0.0147
FLUENT - Park	0.00023	0.607	0.3454	0.04710	4.19×10^{-5}
DS2V - Gupta	0.00103	0.673	0.3013	0.00545	0.0192
DS2V - Park	0.00121	0.671	0.2939	0.01186	0.0188

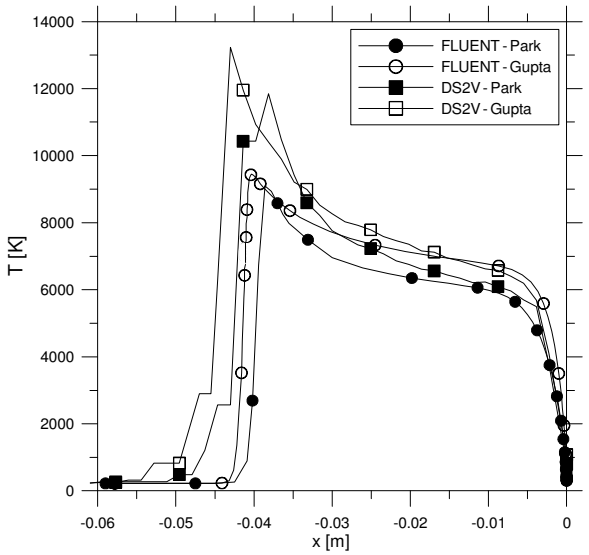

FIGURE 4. Temperature profiles along the stagnation line: non-catalytic surface, h=70 km.

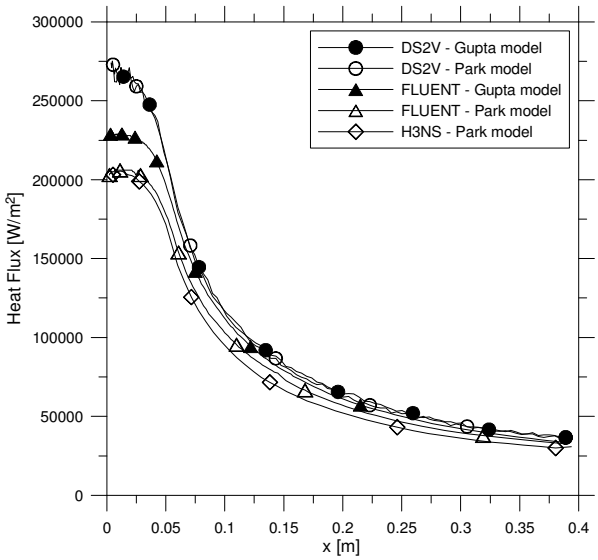

FIGURE 5. Heat flux profiles along the EXPERT nose α=0 deg. predicted by the CFD and DSMC codes non-catalytic surface, h=70 km.

CONCLUSIONS

The chemical models by Gupta and by Park have been compared in the computation fluid-dynamic and direct simulation Monte Carlo codes FLUENT and DS2V. This work completes a former study where the influence of the chemical models by Gupta and by Park on the computation of heat flux on two current capsules was evaluated. Tests were carried out by DS2V and by the CFD code H3NS. DS2V and H3NS use the Gupta and the Park chemical models, respectively. In order to compare the effects of the chemical models, the Park model was implemented also in DS2V. The results showed that DS2V and H3NS compute different compositions both in the flow field and on the surface, even using the same chemical model (Park). Furthermore, DS2V computes, by the two chemical models, different compositions in the flow field but the same composition on the surface, therefore the same heat flux.

In this work, in order to evaluate the influence of the Gupta and the Park models in a CFD code, the models have been tested in FLUENT. Tests by DS2V and by FLUENT have been carried out on the nose of the EXPERT capsule at the altitude of 70 km and with velocity of 5000 m/s. The flow field was hypersonic, continuum low density.

The results showed that FLUENT computes by both chemical models lower values of heat flux, compared with the ones predicted by DS2V. This is justified by a higher reactivity of FLUENT than the one of DS2V. An important different behavior of the two codes, to be pointed out, is that DS2V tends to reduce the differences of the molar fractions by the chemical models toward the surface while FLUENT keeps these differences. As a consequence, the heat flux computation by DS2V is equivalent for both chemical models, on the opposite FLUENT is more sensitive. In fact, at the stagnation point, the heat flux by Gupta is about 13% higher than the one by Park.

Finally, considering that difference in the computation of the heat flux between DSMC and CFD is not negligible, comparing the present computations with the flight data of the Expert capsule will be proper and interesting as well as conducting such kind of comparisons with results by ground based experiments is also important.

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