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SIMULATION OF CHEMICALLY REACTIVE GAS FLOWS AROUND THE SARA CAPSULE: EFFECTS ON THE FLOWFIELD STRUCTURE

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Abstract. *The direct simulation Monte Carlo has been used to study the influence of chemically reactive gas flows around the SARA capsule. In the present investigation, dissociation and exchange reactions was performed using the quantum kinetic chemistry model. This model is solely based on the vibrational states of the colliding molecules and do not require any information about the macroscopic state of simulated molecules. Temperature and density was measured along five different positions normal to the vehicle surface and compared with non-reacting cases. It was found that the chemical reactions promoted a reduction on the temperatures profiles. In addition, during the dissociation process significant amount of atomic oxygen was produced which may lead to an early corrosion of the thermal protection system materials.*

Keywords: *DSMC, Q-K chemistry model, Rarefied gas, Hypersonic flow, SARA capsule*

1. INTRODUCTION

Spacecraft flying at hypersonic speed through Earth's atmosphere are known to produce a large amount of chemical reactions. The chemical reactions products generated during the reentry phase may affect considerably the flowfield surrounding the vehicle, change the heat flux to the surface and aerodynamic loads or even promote an early degradation/erosion of the thermal protections systems (TPS). However, numerical aerothermodynamic prediction is a complicated task which requires robust computational codes to solve problems involving the presence of multiple species and thermochemical nonequilibrium conditions.

Nowadays, the design of hypersonic vehicles relies heavily on computational tools and a significant number of studies have been conducted at different flow regimes. Usually, these numerical investigations are performed using both continuum computational fluid dynamics (CFD) methods and particle methods such as the direct simulation Monte Carlo technique (Moss *et al.*, 2006; Hollis and Borrelli, 2012; Votta *et al.*, 2013; Schmisseur, 2015). Although, for the particular case of the Satélite de Reentrada Atmosférica (SARA) a few investigations have been dedicated to the understanding of its aerothermodynamics (Toro *et al.*, 2001; Sharipov, 2003; Morgenstern and Moraes Jr., 2003; Tchuen *et al.*, 2005; Machado, 2012; Santos, 2012).

Using a thermochemical nonequilibrium Navier-Stokes solver, Tchuen *et al.* (2005) carried out numerical simulations of a hypersonic, seven species, reacting flow over the SARA capsule for Mach numbers ranging from 10 to 25. The results showed good agreement for pressure and heat transfer coefficients when compared to DSMC frozen gas calculations. In addition, the importance of chemical reactions during the re-entry phase of the capsule was emphasize by the authors.

Morgenstern and Moraes Jr. (2003) provided a detailed experimental and numerical numerical investigation of the flowfield in the base region of SARA capsule. The formation of two main vortices characterized by an unsteady flow region was observed. The effect of the unsteady perturbation on the flowfield in the external cylindrical region, where the parachute pressure sensors are located, was the main concern of the study. The numerical solution showed good agreement with the experimental data and a better understanding on the wake flowfield characteristics was achieved.

The impact of 2D and axisymmetric simulations on the the velocity, density, pressure and temperature distributions over the SARA capsule was investigated by Santos (2012). The direct simulation Monte Carlo method was used for non-reacting gas flows at different altitudes, ranging from 80 to 100 km above the Earth's surface. According to his work, a significant difference is observed when the computations is performed using 2D and axisymmetric approaches. It was seen that 2D simulations overpredict the temperature along the profiles causing a significant change on the shock wave structure.

In the present paper, rarefied hypersonic non-reacting and reacting gas flows computations is performed using the direct simulation Monte Carlo technique. The SARA capsule is modeled as a full 3D model at zero angle of attack proving crucial information for the design and fabrication of lightweight and low cost TPS. In order to accomplish this goal, the impact of chemical reactions on the flowfield around the SARA capsule is investigated at an altitude of 95 km.

2. COMPUTATIONAL METHOD

The direct simulation Monte Carlo (DSMC) method has been used over the last 60 years in the numerical investigations of rarefied gas flows (Bird, 1994). It has been developed and improved along these years and successfully applied to the study a wide variety of engineering problems situated in the transition regime (Josyula and Burt, 2011).

The DSMC technique model a gas as a collection of molecules in which one computational molecule represent a large number of real gas molecules. The position, velocity components and internal state of each molecule are stored and modified with time as the molecules collides and interact with boundary conditions. The simulation is always considered as unsteady and the flow properties are determined from the averages of the molecular properties after a very large number of interactions. An important assumption in the DSMC method is that the particle motion and intermolecular collisions are decoupled over small time steps. The time parameter in the flow may be representative of real time and it is advanced according to the collision frequency appropriate for the flow.

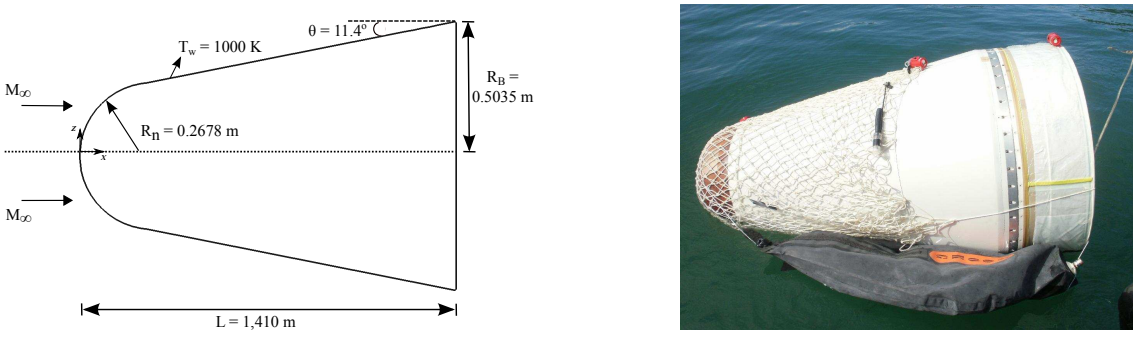
In the present investigation, molecular collision is modeled by using the Variable Hard Sphere model (VHS) (Bird, 1981) and the no-time-counter (NTC) collision sampling technique (Bird, 1989). The energy repartition between translational and rotational mode is controlled by the Larsen-Borgnakke statistical model (Borgnakke and Larsen, 1975) where a fraction φ of the intermolecular collisions is considered as inelastic while the remaining fraction (1 - φ) is treated as elastic. In addition, the rotational relaxation collision number, which corresponds to the number of collisions needed, on average, for a molecule to undergo relaxation, is set equal to 5.

The DSMC code used in the present investigation is called dsmcFoam. The code has been developed within the framework of the open source CFD toolbox OpenFOAM (2015) and it is freely available under the GNU general public license. The main features of the dsmcFoam code include the capability to perform both steady and transient DSMC simulations, perform simulation employing arbitrary two- and three-dimensional geometries using unstructured polyhedral meshes and unlimited parallel processing. The code has been successfully benchmarked against numerical and experimental data available in the literature for non-reacting gas flows (Scanlon *et al.*, 2010; Palharini *et al.*, 2015).

As discussed earlier, chemical reactions is of fundamental importance on the correct estimation of aerodynamic and thermal loads acting on the reentry vehicle surface. The first chemical reactions model employed in the DSMC method was proposed by Bird in 1979 and it is known as the total collision energy (TCE) model (Bird, 1979). This model relies upon input data derived at the macroscopic level and reaction rate coefficients that are derived from equilibrium theory and it has been used in mature DSMC codes (Boyd, 2007). More recently, Bird (Bird and Abe, 2009; Gallis *et al.*, 2009) recommended a molecular-level chemistry model that predict equilibrium and nonequilibrium reaction rates using only the kinetic theory and fundamental microscopic properties of the gas. This new chemistry model, called quantum-kinetic (Q-K) chemistry model, does not use any macroscopic rate information and it just depends on vibrational collision number, which is a function of the collision temperature. In this new chemistry model vibrational energy can only assume discrete quantum values (Haas *et al.*, 1993; Bergemann and Boyd, 1992) and a serial application of the quantum Larsen-Borgnakke method is used to redistribute vibrational energy before rotational and translational energy exchange (Scanlon *et al.*, 2015). In the present paper, a 5-species (oxygen O_2, nitrogen N_2, nitric oxide NO, atomic oxygen O, and atomic nitrogen N) Q-K chemistry model is used to investigate the impact of dissociation and exchange reactions on the flowfield structure around the SARA capsule during the reentry phase.

3. CAPSULE GEOMETRY AND REENTRY CONDITIONS

A detailed representation of the Brazilian Reentry Satellite is shown in Fig. 1. SARA was designed based on the cone-sphere configuration in which the nose radius (R_{nose}) is 0.2678 m and 11.4° half-angle conical afterbody (Santos, 2012). The total length of the capsule is set as 1.410 m with a base radius of 0.5035 m. All the simulations was performed at 0° angle of attack, i.e., the incoming freestream is parallel to the X-axis.



(a) (b)

Figure 1. Schematic of SARA main parameters (a) and capsule during the floating test (b).

The freestream conditions addressed here correspond to those experienced by the Brazilian reentry capsule at 95 km altitude. The main flow features can be accessed in the U.S. Standard Atmosphere tables (NOAA/NASA/USAF, 1976) and for the particular altitude investigated these informations are tabulated in Tab. 1. In addition, the flow conditions showed in Tab. 1 were used to perform both reacting and non-reacting computations. At 95 km altitude, the atmosphere is composed by 78.351% N_2, 20.141% O_2, and 1.508% O. The the freestream mean free path, λ_∞, was determined by the variable hard sphere molecular model (Bird, 1983). The overall Knudsen number, Kn, is defined as the ratio of the molecular mean free path to a certain characteristic dimension. Considering the SARA's nose radius as the characteristic dimension the Knudsen number correspond to 0.153 and lies in the transition regime. The Reynolds number, $Re_{R_{nose}}$, based on the freestream conditions and calculated considering the nose radius as the characteristic length correspond to a value of 232.71, i.e., hypersonic laminar flow. The reentry velocity was set at 7860 m/s for the dsmcFoam computations and established based on the velocity-altitude-map presented by Pessoa Filho (2008).

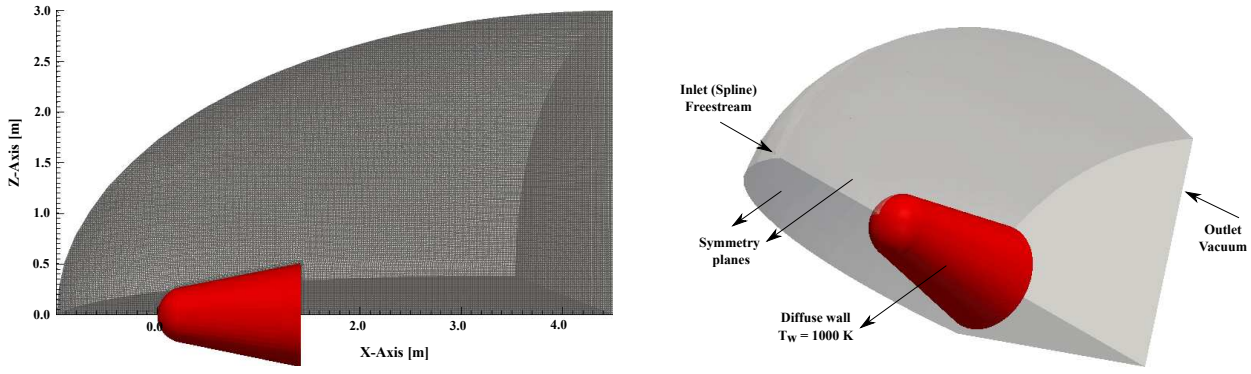
Table 1. Freestream flow conditions experienced by the SARA capsule at 95 km altitude.

Parameters	Mach	U_∞ [m/s]	T_∞ [K]	n_∞ [m^{-3}]	ρ_∞ [kg/m^3]	p_∞ [Pa]	λ_∞ [m]
Values	28.45	7860	188.42	2.92×10^{19}	1.39×10^{-6}	7.53×10^{-2}	4.11×10^{-2}

4. COMPUTATIONAL DOMAIN AND BOUNDARY CONDITIONS

In the present investigation, advantage was taken from SARA's axisymmetry in order to reduce the computational costs. The computational mesh was prepared using a quarter-section model with symmetry boundary condition, as depicted in Fig. 2. For the altitude considered, a cubic mesh of $275\times150\times150$ cells was employed covering a domain size of 5.5 m in the flow direction and 3 m in the z- and y-directions. The OpenFOAM mesh utility called $snappyHexMesh$ was used to 'snap' the mesh on to the SARA CAD geometry creating hexahedral cells onto the surface. After this process, a total of 3.2 million cells were used in the dsmcFoam calculations.

The computational mesh was filled with 64.3 million DSMC particles. Freestream conditions were applied at the inlet of the computational domain, represented as a spline in Fig. 2b). The flow at the downstream outflow boundary is supersonic and vacuum conditions were specified (Bird, 1994). For all computations, the outflow boundary was located 4.5 m downstream of the forebody stagnation point. The two perpendicular planes on the side of the capsule represents the symmetry planes, where all flow gradients normal to the plane are zero. At the molecular level, this boundary condition is equivalent to a specular reflecting wall. The wall temperature was kept constant at 1000 K with the gas-surface interaction being modeled diffusively with full thermal and momentum accommodation.



(a) (b)

Figure 2. 3D SARA computational domain (a) and boundary conditions (b).

5. COMPUTATIONAL RESULTS

This section aims to discuss the impact of chemically reactive hypersonic gas flows on the temperature and density profiles around the SARA capsule. Five different normal profiles are analyzed where their length is measured from the vehicle's surface to inlet boundary condition and normalized by the capsule nose radius (R_{nose}). In addition, the profile starting point is given by the ratio of the x-direction position at wall and capsule nose radius (S = x/R_{nose}).

5.1 Temperature Field

As a consequence of the strong shock wave formed upstream of a hypersonic vehicle during the reentry phase, the high kinetic energy present in the flow is rapidly converted to thermal energy. This high temperature region may promote the dissociation and possible ionization of the air surrounding the capsule leading to a significant impact on the flowfield structure.

In order to study the impact of chemical reactions on the flowfield structure around the SARA capsule, Figure 3 presents the temperature distribution along five different profiles positioned perpendicularly to the vehicle surface. Profile 1 represents the temperature distribution along the stagnation streamline, P_2 and P_3 are located in the capsule blunted nose and P_4 and P_5 are positioned at the SARA conical body. The translational, rotational and vibrational temperatures was measured from the capsule surface (S) to the inlet boundary condition. The temperatures along the profiles were normalized by the freestream temperature (T_∞) and the profile length was normalized by the capsule nose radius. In this set o plots, full symbols shows the simulations performed using the Q-K chemistry model (dsmcFoam-QK) and empty symbols correspond to non-reacting gas flows computations (dsmcFoam-NR).

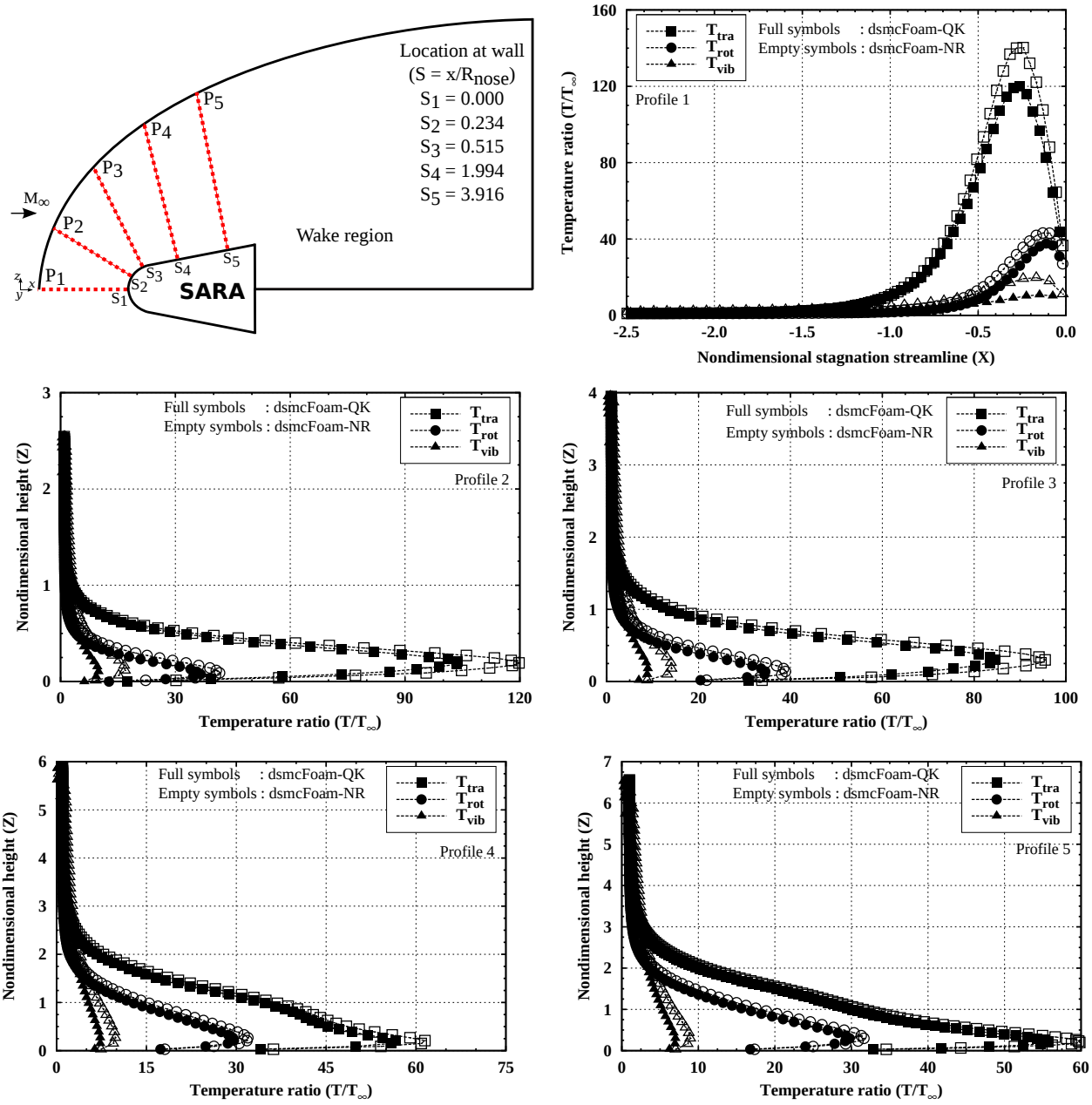


Figure 3. Temperature ratio (T/T_∞) distribution along five different profiles normal to SARA surface for reacting and non-reacting air flow.

According to Figure 3, it is clear seen that the chemical reactions led to a significant reduction on the temperature ratio along the profiles considered. Along the profile P_1, the translational and internal temperatures have the same value far from the vehicle nose. However, as the molecules approaches the stagnation point the translational temperature is increased and its maximum value occurs location X=-0.28. In addition, due the endothermic feature of the chemical reactions, a reduction of 17%, 14.3% and 81.5% is observed for translational, rotational and vibrational temperatures, respectively.

From temperature profiles 2 to 5, it is observed that the difference on the temperature peak inside the shock layer for reacting and inert gas flow decrease as the flow moves downstream along the body surface. The reduction on translational temperature ratio (T_{tra}/T_∞) at P_2 was 15.3% when all chemical reactions is activated and at P_5 the temperature diminution was of the order of 7.3%.

5.2 Density Field

As previously demonstrated, chemical reactions play a very important role on the reduction of flow temperature around the SARA capsule. The reduction of the flow temperature is mainly caused by the endothermic reactions where part of the flow energy is absorbed by air molecules and employed in the dissociation process. The dissociated molecules generate new species as atomic oxygen/nitrogen and nitric oxide leading to a significant change on the flow composition around the spacecraft. In this way, the impact of chemical reactions on the density distribution for each specie is presented in Figures 4 to 6.

Figure 4a) and 4b) illustrate the density ratio (ρ/ρ_∞) along the entire stagnation streamline and in a region close to the SARA spherical nose, respectively. Similarly to temperature distribution, the density profiles were normalized by the freestream density (ρ_∞) and the profile length was normalized by the capsule nose radius. By comparing the species density ratio along the stagnation streamline for molecular nitrogen, N_2 density ratio is high close to the SARA surface and decreases as the inlet boundary is approached. Furthermore, as the energy necessary to fully dissociate the molecular nitrogen is considerably high, no significant change on the nitrogen density ratio was observed for SARA reentry at 95 km altitude. Furthermore, as dissociation reactions take place at the high temperature region close to the SARA spherical nose, it is noticed a decrease on the O_2 density ratio and an significant increase of atomic oxygen/nitrogen and nitric oxide.

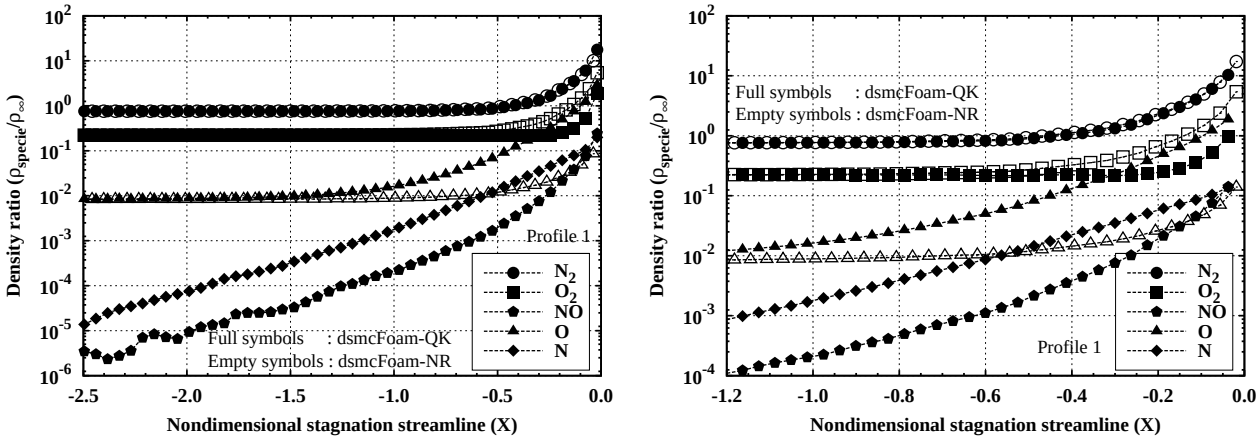


Figure 4. Density ratio (ρ/ρ_∞) distribution along the stagnation streamline for reacting and non-reacting air flow around the SARA capsule.

In order to deeply understand the impact of chemical reactions on the flowfield structure, Figs. 5 and 6 presents the density distribution for O_2 and O separately for each profile. It is observed from Figure 5 a expressive difference on the O_2 and O density ratio profiles for reacting (dsmcFoam-QK) and non-reacting (dsmcFoam-NR) gas flows around the capsule. In a region which varies from X = 0 to X = -5 along the stagnation streamline, a reduction of 187.3% on the molecular oxygen is noticed. In the shock layer, kinetic energy of the air flow is converted to heat and dissociation reaction still occurring as the flow moves around the capsule. The molecular oxygen density ratio is high close to the wall, Z = 0; however, the difference on the maximum O_2 concentration for reacting and inert gas flows at P_5 is 44.34%.

Finally, Figure 6 show the atomic oxygen density ratio (ρ_O/ρ_∞) distribution at five different positions normal to the SARA surface. According to this group of plots, a significant increase on the atomic oxygen close to the wall is observed in all profiles investigated. Along the profile P_1, the raise of atomic oxygen start to happen at location X = -1.6 and its maximum value is reached at the stagnation point. Due to O_2 dissociation inside the shock wave producing atomic oxygen, the O concentration at this region is 21 times higher for reacting gas flows. Even with the flow expansion over the vehicle, the O density ratio at P_5 is 743.4% higher for chemically reactive gas flows.

6. CONCLUSIONS

Numerical investigation of rarefied hypersonic flow around the SARA capsule has been conducted using the direct simulation Monte Carlo technique. Simulations were performed using the Q-K chemistry model and the results were compared with non-reacting calculations. This study provided important information on the impact of chemical reactions in the temperature and density profiles normal to the vehicle surface.

The analysis showed a significant reduction on the temperature close to the vehicle surface when chemically reactive gas flows is considered. In addition, due the dissociation of the molecular oxygen promoted in the forebody shock wave, the atomic oxygen concentration is 21 times higher when compared with inert gas flows. This difference is reduced to 743.4% at P_5 as the flow expands around the vehicle. It is worth to notice that atomic oxygen is one of the main sources of premature corrosion of thermal protection system materials and high concentration of this atomic specie close to the vehicle may significantly increase the erosion the material used to protect the capsule during a severe reentry.

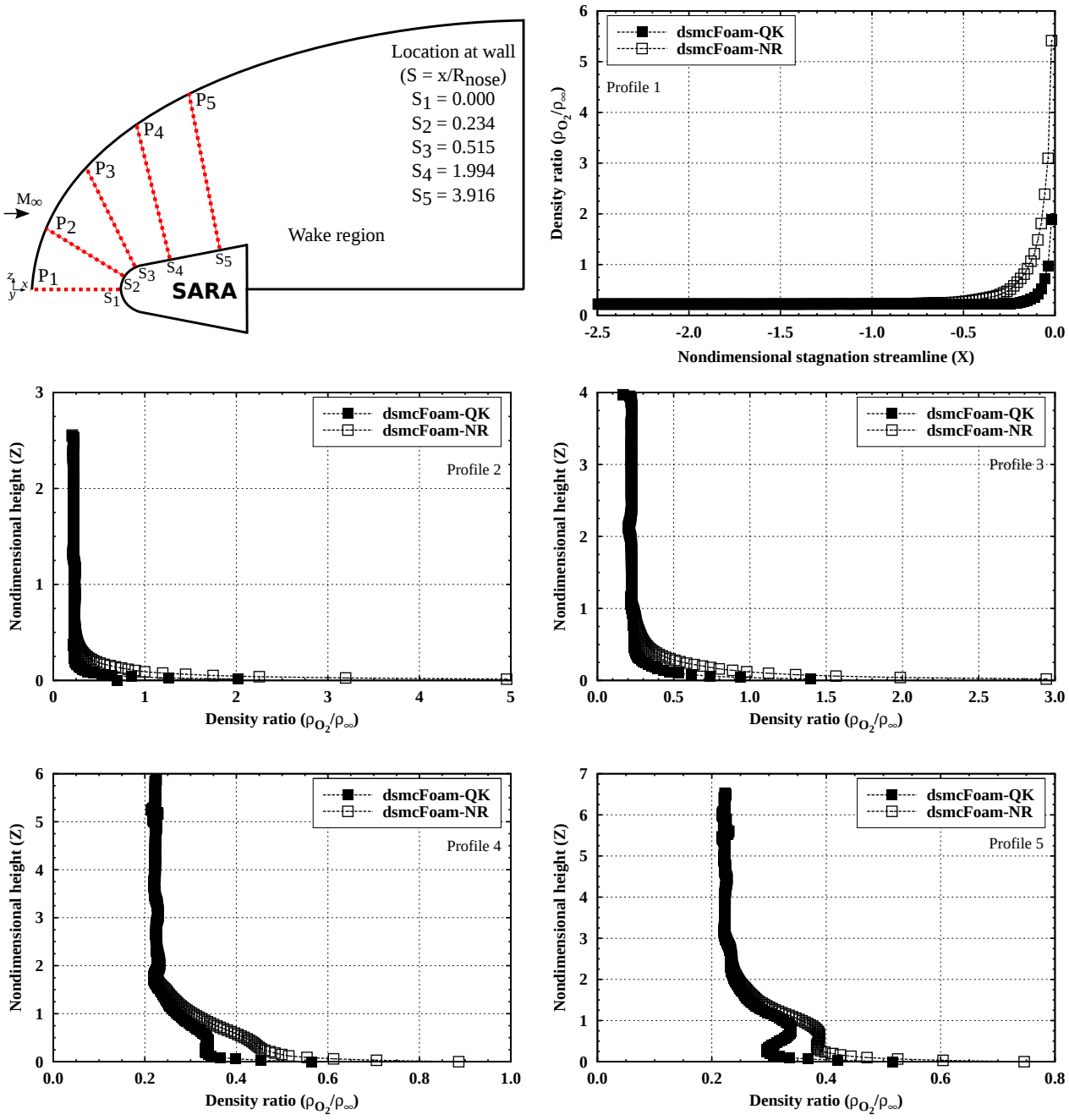


Figure 5. Molecular oxygen density ratio (ρ_{O_2}/ρ_∞) distribution along five different profiles normal to SARA surface for reacting and non-reacting air flow.

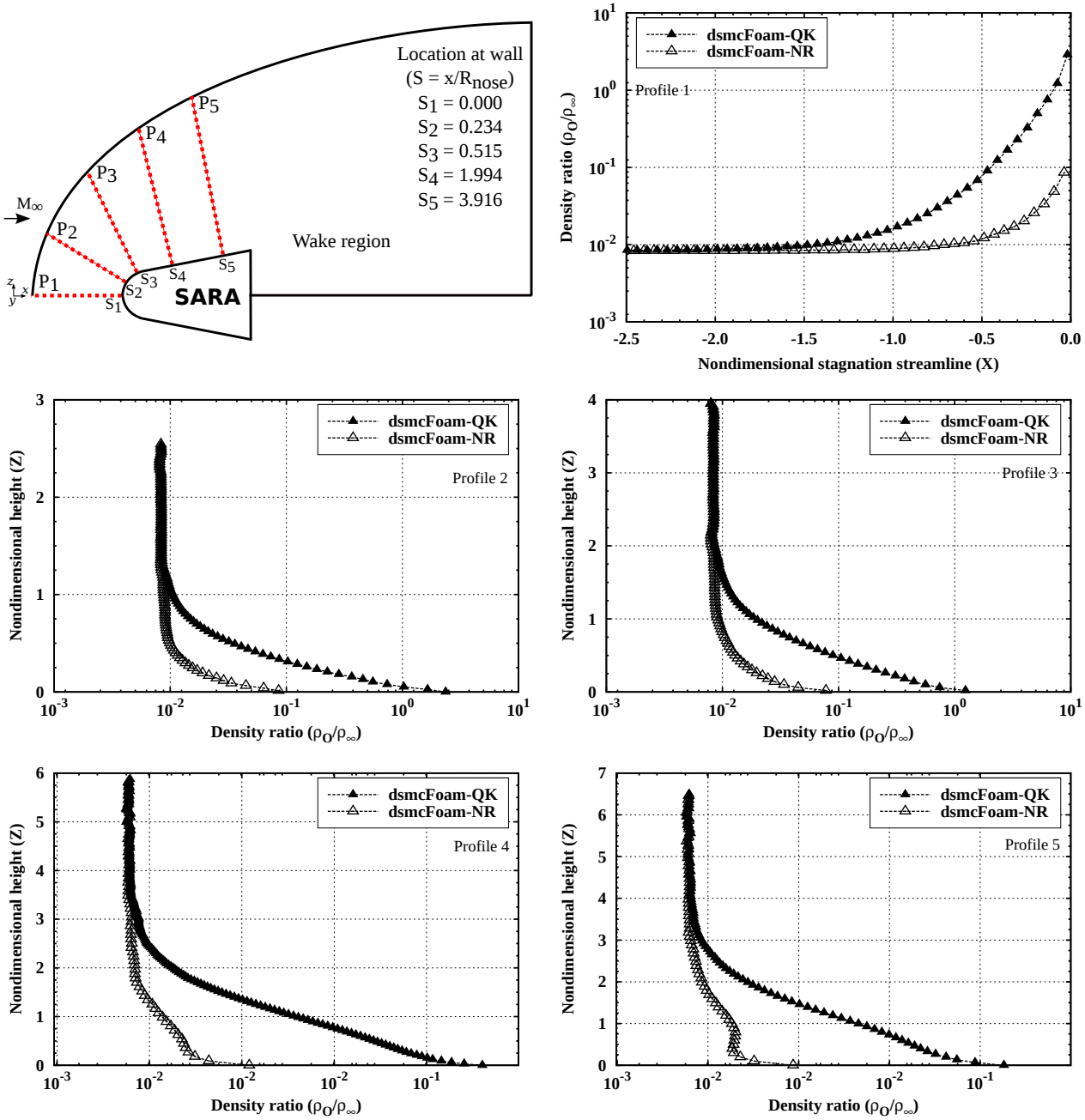


Figure 6. Atomic oxygen density ratio (ρ_O/ρ_∞) distribution along five different profiles normal to SARA surface for reacting and non-reacting air flow.

7. ACKNOWLEDGEMENTS

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