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AXISYMMETRIC RAREFIED FLOW AROUND A BLUNTED BODY: NUMERICAL AND EXPERIMENTAL COMPARISON

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Abstract. *The current paradigm of space exploration includes the growing demand for missions to other planets and the utilization of reusable vehicles. To achieve these goals, numerical simulation tools are needed to predict aerodynamic and aerothermodynamic parameters in different flight regimes. Although, some care must be taken because, specifically under rarefied atmosphere conditions, the continuum hypothesis is not valid. Under these rarefied conditions, traditional Computational Fluid Dynamics (CFD) models are not physically accurate and predictions must be made using tools capable to account the discrete nature of the gas. The widely used of these tools in engineering applications is the Direct Simulation Monte Carlo (DSMC). However, despite their accurate results, DSMC simulations require large computational resources. To decrease the computational cost for DSMC simulations an axisymmetric version of the DSMC method implemented in the OpenFOAM software was recently developed. Here, the axisymmetric DSMC was applied to the simulation of rarefied hypersonic flow conditions around a blunt body. The simulation results were compared with 3D dsmcFoam calculations and wind tunnel data available. The results showed a good agreement between the 3D and the axisymmetric DSMC calculations, with both numerical simulations having good agreement with the experimental data. In the axisymmetric code, there was a decrease in the processing time of results during numerical simulations. The axisymmetric formulation is roughly 127 times faster compared to the 3D DSMC code.*

Keywords: *Direct Simulation Monte Carlo, Aerothermodynamics, Rarefied Flows, Axisymmetric Simulation*

1. INTRODUCTION

The atmospheric reentry of a space vehicle is one of the most critical phases during its mission, considering its exposure to high-speed flow and high temperature conditions (Palharini, 2014). In the circumstance of crescent space exploration demanding for reusable vehicles, adequate prediction of the flow behavior around these vehicles is vital for the design of thermal protection systems in order to safeguard the payload in hostile reentry conditions (Martin, 2011).

In this context, the Brazilian Aeronautics and Space Institute is developing studies on the use of numerical tools capable of accurately calculating the aerothermodynamics of reentry vehicles under different flow conditions. Therefore, it is necessary to measure the validity of numerical codes available, to cover the entire spectrum of environmental conditions swept by the reentry trajectory of a space vehicle.

The main parameter used in these conditions is the Knudsen number, a dimensionless parameter that measures the degree of rarefaction of the flow as,

$$Kn = \frac{\lambda}{L} \tag{1}$$

where the molecular mean free path λ is compared to the characteristic length scale L of the system under consideration. Knudsen numbers lower than 0.1 guarantee adequate results from numerical methodologies of Computational Fluid Dynamics (CFD). On the other hand, problems in which the study domain has vast regions with high degrees of rarefaction, evidenced by Knudsen numbers greater than 0.1, require numerical modeling based on the particle nature of matter, such as the Direct Simulation Monte Carlo (DSMC) (Bird, 1994).

In the DSMC method, the dynamics of the particles are calculated under the assumption of the decoupling between the particle advection and the inter-particle collisions inside the cells, which implies that the time step should be chosen to be sufficiently small in comparison to the local mean collision time (Hadjiconstantinou (2000), Garcia and Wagner (2000)).

An additional requirement of the method is the minimum number of simulated particles employed in the numerical cells. As the system evolves towards quasi-equilibrium through particle collisions, the relaxation rate is dependent on the number of particles in the cells, so that it is theoretically desirable that each cell has the largest possible number of particles. However, as stated by Bird (1994), from the numerical point of view it is necessary to determine an optimum number of particles per cell, so that the flow dynamics is statistically well represented, while maintaining an achievable computational cost. To solve these requirements, Bird (1987) introduced the procedure of subdividing the cells into an arbitrary number of sub-cells for the selection of collision pairs, ensuring that collisions occur only between near-neighbor particles, improving the accuracy of the method. Results showed that the minimum required number of particles in each cell is between 20 to 30 particles.

Despite its accurate results, 3D DSMC simulations require high computational resources. Thus, the main objective of the present work is to evaluate the numerical performance gain compared to 3D simulations and to validate the axisymmetric results compared to experimental wind tunnel data from Allegre et al (1997). Here, a rarefied hypersonic flow around a blunt body was performed and the results were compared to 3D dsmcFoam computations and wind tunnel experimental data available.

2. COMPUTATIONAL METHOD

2.1 DSMC Code

The DSMC is a stochastic particle numerical method build upon kinetic theory and loosely based on the Boltzmann equation. The method was developed by Bird between 1960 and 1980, becoming a reference in terms of numerical prediction tool to study the aerothermodynamics of rarefied flows (Cercignani, 2000). Although the DSMC method is not derived directly from the Boltzmann equation, Wagner (1992) showed that, in the limit of a vanishing discretization error, steady state DSMC calculations converged to the solutions of the Boltzmann equation. Moreover, being based on the classical kinetic theory, the DSMC is controlled by the same restrictions of the Boltzmann equation, i.e., assumption of molecular chaos and restrictions related to dilute gases, where the mean molecular diameter is much smaller than the mean molecular space in the gas.

According to Boyd and Schwartzentruber (2017), the dilute gas hypothesis guarantees three physical assumptions that enables the DSMC method to simulate, using a reduced number of particles, macroscopic nonequilibrium flow fields around generic geometries, (1) Molecules moving in free flight without interaction for time scales on the order of the local mean collision time; (2) The impact parameters and initial orientations of colliding molecules are random; and (3) There are an enormous number of molecules per cubic mean free path and only a small fraction need to be simulated to obtain an accurate description of the flow.

For the first assumption, Boyd and Schwartzentruber (2017) explain that there can be many millions of particles contained within each cubic mean free path, implying that each molecule experiences, on average, only one collision as it moves across this volume. Being dilute assures that the particles of the gas have separation distance between each other much greater than the extent of intermolecular forces and therefore molecules do move in straight lines, in a free flight, for a fraction of their mean collision time. The numerical accuracy of the assumption (1) was observed in the Molecular Dynamics (MD) simulations made by Valentini and Schwartzentruber (2009).

The second assumption was also corroborated by MD simulations, which the impact parameters and particle orientations of colliding molecules in a dilute gas are completely random. This also explains why the collisions in the DSMC method do not need to be deterministically simulated as they are in the MD method (Boyd and Schwartzentruber, 2017).

Finally, the third physical assumption is based on stochastic arguments, since that it is not necessary to simulate the properties of all real particles in each mean free path cubic volume. Figure 1, adapted from Boyd and Schwartzentruber (2017), shows two types of real particles that lie within, respectively, the two same narrow ranges in the velocity distribution function. So, instead of simulating each particle, tracking its position and velocity, it is possible to simulate a much smaller number of particles, called DSMC particles, that represents a large number of real particles that restitutes the distribution function of the physical flow field.

It is important to know that DSMC particles do not represent a distribution of real molecules, but represent a large number of identical real molecules. This enables collisions between pairs of simulated particles to be modeled with precisely the same physical considerations as collisions between pairs of real molecules (Boyd and Schwartzentruber, 2017). However, a few DSMC particles does not have the deterministic nature of millions of real particles, even though their simulation restitutes accurately the distribution functions in the spatial and temporal scales of the mean free path and mean collision time, respectively.

The lack of deterministic representation of real molecules throughout the scales below the DSMC cell dimension explains the choice of performing collisions in a probabilistic way. During each time step, DSMC particles are randomly paired up within each cell, and subsequently tested for a collision. Thus, as described in Boyd and Schwartzentruber (2017), all possible collision pairs, consisting of all classes of molecular velocities, internal energies, and chemical species, are sampled in a Monte Carlo fashion from the actual distributions of particles within each cell. In fact, the distance between two DSMC particles inside the same DSMC cell does not determine whether they collide or not, it is possible the two representative DSMC particles in the left square of the Fig. 1 collide with each other, despite their velocity vectors are not pointing toward each another.

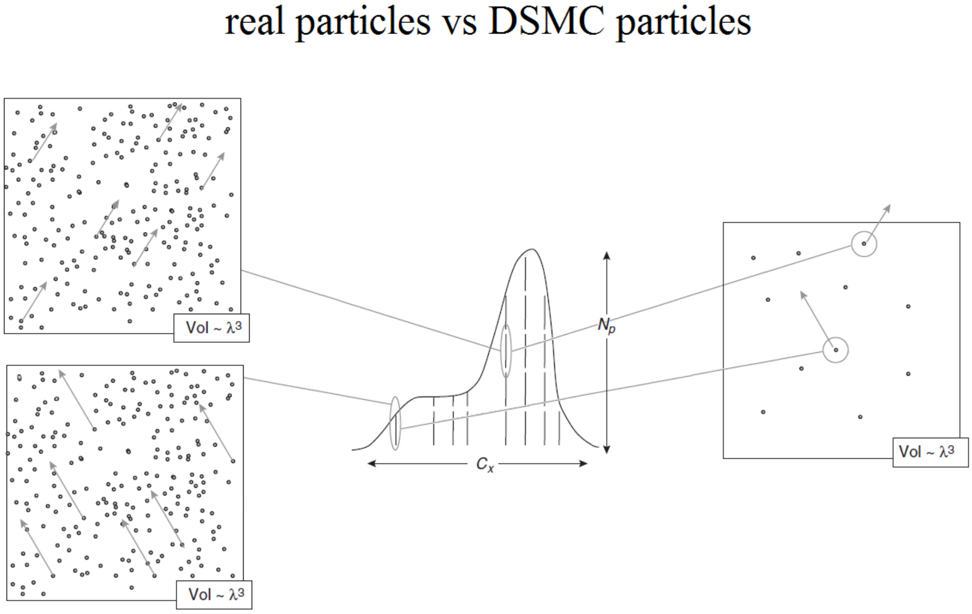

Figure 1. Schematic characteristics of the DSMC method (adapted from Boyd and Schwartzentruber, 2017).

The DSMC algorithm mimics molecular dynamics models in the sense that the state of the system is calculated from the degrees of freedom of N particles, so that state of the particles is given by (Bird, 2014),

$$X(t) = (\vec{r}_1(t),\ldots,\vec{r}_N(t),\vec{p}_1(t),\ldots,\vec{p}_N(t),e_1(t),\ldots,e_N(t)), \tag{2}$$

where $\vec{r}_j(t)$, $\vec{p}_j(t)$ and $e_j(t)$ are the position vector, the momentum vector and the internal degrees of freedom, respectively, for the particle j, with $j = 1,\ldots,N$. As described by Palharini (2014), the state of each particle is stored and modified with time as the particle moves, collides and interacts with the surface in the simulated physical domain obeying the rules of kinetic theory.

To assure proper physical behavior for the DSMC particles, the DSMC algorithm sorts particles into numerical cells, such that only particles in the same cells have a nonzero collision probability that depends on the interaction model being used. Generally, the collision probability between particles m and n can be calculated as,

$$P_{mn} = F_N\, \sigma_{mn} c_{r,mn} \Delta t\, V_C, \tag{3}$$

where the probability P_{mn} of collision between DSMC particles m and n, depends on the statistical weight F_N , the impact collision cross section σ_{mn} , the relative velocity magnitude $c_{r,mn}$, the time step Δt and the cell volume V_C. After selection, the particle pair is tested for collision using an acceptance-rejection method (Bird, 1994), where the pair is accepted for collision if,

$$(\sigma_{mn} c_{r,mn})/(\sigma c_r)_{\max} > R_u, \tag{4}$$

with $(\sigma c_r)_{\max}$ the maximum of the product between the impact collision cross-section and the particles relative speed, for all particles in the cell, and $R_u$is a random number uniformly distributed in the interval from 0 to 1.

After a collision takes place, linear momentum and energy conservation requirements dictate the post-collision dynamics of the DSMC particles. Following Alexander and Garcia (1997) and White et al (2017), linear momentum stipulates that the centre of mass velocity $\vec{v}_{CM,mn}$, remains constant, so that

$$\vec{v}_{CM,mn} = (m_m\vec{v}_m + m_n\vec{v}_n)/(m_m + m_n) = (m_m\vec{v}_m^* + m_n\vec{v}_n^*)/(m_m + m_n) = \vec{v}_{CM,mn}^*, \tag{5}$$

where the * symbol represents post-collision properties. Energy conservation, otherwise, implies that the magnitude of the relative velocity is kept constant,

$$c_{r,mn} = |v_m - v_n| = |v_m^* - v_n^*| = c_{r,mn}^*. \tag{6}$$

Using the two conservation laws and the scattering angles, it is possible to find a solution for $c_{r,mn}^*$. The scattering of the elevation angle and the azimuthal angle is dependent on the interaction model being used. For a variable hard sphere (VHS) model, for example, these angles are distributed over a unit sphere, such that the azimuthal angle φ is uniformly distributed between 0 and 2π and the elevation angle θ is uniformly distributed in the real interval from -1 to 1, with

$$\varphi = 2\,\pi\,R_u \qquad \cos\theta = 2R_u - 1 \tag{7}$$

where $R_u$being a random number uniformly distributed in the interval from -1 to 1.

Finally, the three components of the post-collision relative velocity and the post-collision velocities for the particles m and n become are calculated as

$$\vec{c}^{\,*}_{r,mn} = c^{*}_{r,mn}\,(\cos\theta\,\hat{x} + \sin\theta\cos\varphi\,\hat{y} + \sin\theta\sin\varphi\,\hat{z}) \qquad \vec{v}^{\,*}_{m} = \vec{v}_{CM,mn} + (m_n/(m_m+m_n))\vec{c}^{\,*}_{r,mn} \qquad \vec{v}^{\,*}_{n} = \vec{v}_{CM,mn} + (m_m/(m_m+m_n))\vec{c}^{\,*}_{r,mn} \tag{8}$$

Due to the stochastic nature of the method, results obtained from DSMC simulations must be sampled for the calculation of the macroscopic flow properties. Thus, the computational cells used for selecting the collision pairs are also used as a reference domain for the sampling of the macroscopic gas properties, as long as the linear dimensions of the cells are held small in comparison with the length of the macroscopic flow gradients normal to the streamwise directions, which means that the cell dimensions should be the order of or smaller than the local mean free path (Bird (2014), Alexander et al. (1998), Alexander et al. (2000)).

2.2 Axisymmetric Simulation

The simulation requirements outlined above can lead to prohibitive computational costs for full three-dimensional calculations. An alternative approach to overcome this issue is the application of axially symmetric computations. The DSMC algorithm for axially symmetric flows is similar to the two-dimensional formulation, so that the computational model employs two independent spatial variables, but instead of modeling a unit width dimension the full azimuth about the axis of symmetry is taken into account (Bird, 2014).

However, dsmcFoam computations of axially symmetric flows require the usage of a wedge domain of a small angle, which imposes practical problems for these computations, as there will be a huge imbalance in the fraction of molecules that occupies the outermost cells and the cells located near to the axis of symmetry.

To solve this limitation, Bird (1994) introduced a method to balance the particle distribution into the cells, called Radial Weighting Factor (RWF), where a particle at greater radial distance represent more real particles than a particle located near the axis. This implies that along the particles trajectories some of them will be duplicated or discarded to maintain the even number of particles per cell, through,

$$RWF(r) = 1.0 + maxRWF\left(\frac{r}{R_{ext}}\right) \qquad P_u = RWF_{old}/RWF_{new} - 1 \tag{9}$$

where $maxRWF$ is the maximum value of the radial weighting factor set by the user, r is the radial position of the DSMC particle and R_{ext} is the maximum radial extent of the domain, also set by the user, RWF_{old} (or RWF_{new}) is the radial weighting factor of a DSMC particle before (or after) the movement stage and P_u is the calculated probability. If a DSMC particle moves in the radial direction they have a probability of being deleted (if moving away from the radial centre), or being duplicated (if moving towards the radial centre) (MNF, 2018a). If that probability P_u is greater then 1, that means the DSMC particle is moving towards the axis, so it will be duplicated, if it is smaller then 1, than the DSMC particle is moving outwards the axis, so it will be deleted, (MNF, 2018b).

2.3 dsmcFoamPlus Implementation

The DSMC code to be used in this study is the dsmcFoamPlus (White et al, 2017), a derivation of the dsmcFoam that has been written within the framework of the open-source C++ CFD toolbox OpenFOAM (Scanlon et al., 2010). The main features of the dsmcFoam code include the capability to perform both steady and transient DSMC simulations for multi-species conditions, to model arbitrary 2D/3D geometries using unstructured polyhedral meshes, and unlimited parallel processing. The original version of dsmcFoam determines intermolecular collisions for polyatomic species using the VHS model (Bird, 2014) and applies the phenomenological Larsen-Borgnakke model to distribute post-collision energy between the translational, rotational, and vibrational modes (Bird, 2014). A series of successful benchmark trials have been carried out which have validated the dsmcFoam code for non-reacting and reacting gas flows (Scanlon et al., 2010). The dsmcFoamPlus release of the code includes many features not found in standard dsmcFoam, such as simulation axisymmetric geometries, chemical reactions and subsonic pressure boundary conditions (White et al, 2017).

3. SIMULATION PROPERTIES

The flow over blunt bodies at high speeds and high altitudes is associated with complex flow interactions and the precise determination of the heat transfer fluxes, aerodynamic forces, the topology flow surrounding the spacecraft, as well as the characterization of the wake region are key factor for the success of a re-entry mission (Palharini, 2014).

In the present work, it was simulated a rarefied hypersonic flow around a 70-degree spherically blunted cone with forebody configuration identical to that of the Mars Pathfinder probe. That configuration was chosen due to the large collection of experimental data available in the literature. A series of experiments was simulated for this configuration was performed in the SR3 wind tunnel at Centre National de la Recherche Scientifique (CNRS-Meudom), with test conditions available in AGARD (1996). Particularly, Allegre et al (2017a, 2017b and 2017c) provided detailed information of the 70-degree blunted cone experiments conducted in the SR3 low-density wind tunnel.

Simulation configurations employed the Mars Pathfinder probe immersed in a nonreacting nitrogen gas uniform flow with energy exchange allowed between the translational, rotational and vibrational modes. The energy exchange between the kinetic and internal modes was controlled by the Larsen-Borgnakke statistical model (Cercignani, 2000). The molecular collision kinetics were modelled by the VHS model and the no time counter (NTC) collision sampling technique (Bird, 1994). Details of freestream conditions for the present work are shown in Table 1. For the axisymmetric simulation, the simulation parameters are shown in Table 2. A time discretization smaller than the mean collision time and one fifth of the averaged residence time of a molecule in a cell (Palharini, 2014). For the spatial discretization, it is used a cell with a dimension of one third of the mean free path recommended by Bird (1994).

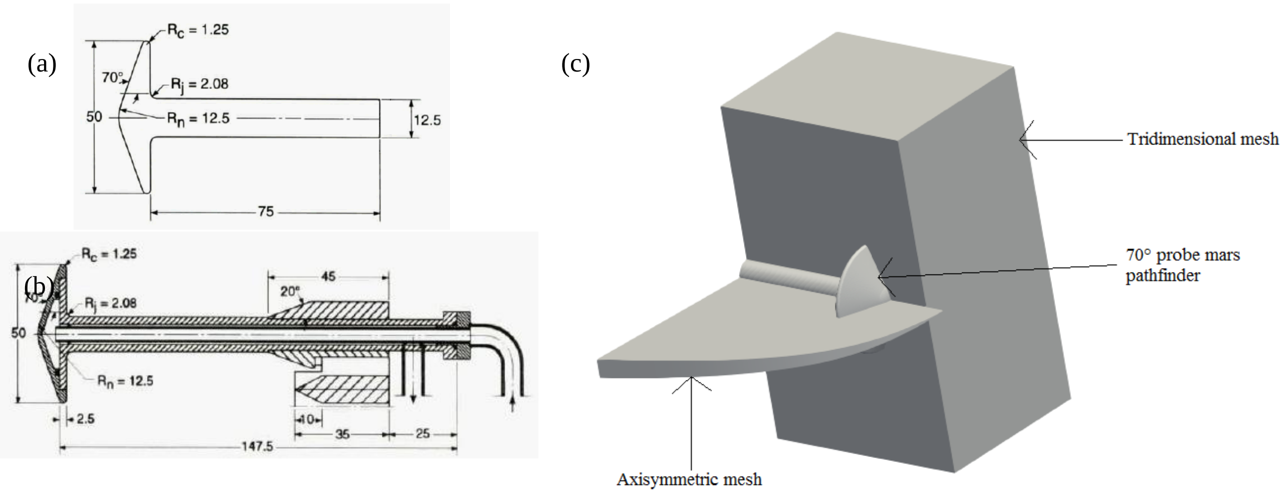

Figure 2. (a) Dimensions in millimeters of the model simulated in the present work, (b) Experimental model for near-wake density mappings in the CNRS (AGARD, 1996) and (c) Three-dimensional computational domain used by Palharini (2014) compared to the axisymmetric domain used in the present work.

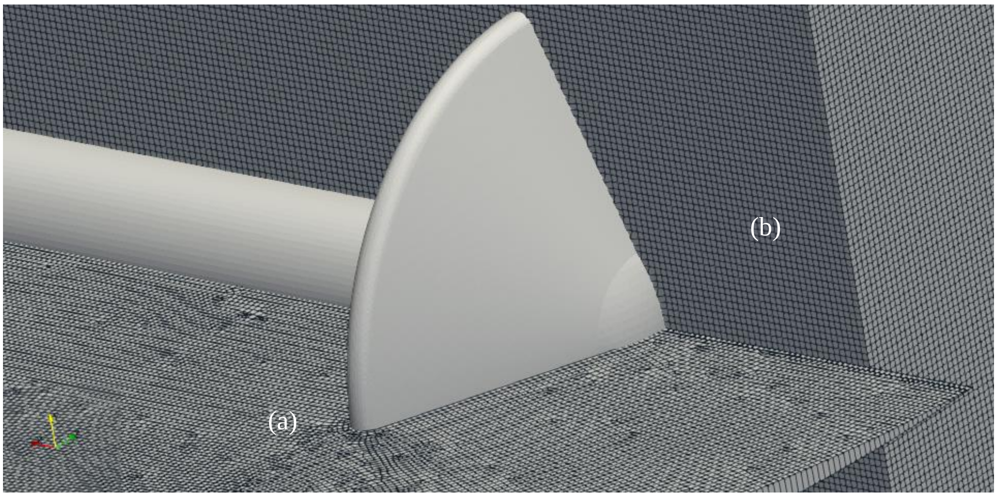

Figure 3. Detailed view of (a) the axisymmetric and (b) three-dimensional meshes, with same cell size but, respectively with 29352 and 7125852 cells.

The experimental model configurations are shown in Figures 2(a) and 2(b). Figure 2(c) presents information of the axisymmetric dsmcFoamPlus mesh compared with the tridimensional one used by Palharini (2014). The axisymmetric computational mesh was composed by 29352 elements with 20 simulated molecules per cell, meanwhile the tridimensional mesh used by Palharini (2014) was composed by 7125852 elements with 10.5 simulated molecules per cell.

Table 1. Freestream conditions for the Mars Pathfinder Simulation.

Parameter	Symbol	Value	Unit
Velocity	V_∞	1503	m/s
Temperature	T_∞	13.3	K
Number Density	n_∞	3.717×10^{20}	m^{-3}
Density	ρ_∞	1.730×10^{-5}	kg/m^3
Pressure	p_∞	6.833×10^{-2}	Pa
Mean Free Path	λ_∞	1.691×10^{-3}	m
Overall Knudsen	Kn_∞	0.034	$-$
Reynolds Number	Re_∞	178.6	$-$

Table 2. Present work axisymmetric dsmcFoamPlus simulation parameters.

Parameter	Symbol	Value	Unit
Time discretization	$\Delta t = \Delta t_{res}/5$	6.82×10^{-8}	s
Spatial discretization	$\Delta x = \lambda/3$	5.64×10^{-4}	m
Molecules per cell	$molec/cell$	20	$-$
Equivalent Number	n_{eq}	4.62×10^{7}	$-$
Simulation time	$T_{500.000\ iterations}$	239316	s

4. RESULTS

Figure 3 shows the axisymmetric dsmcFoamPlus simulation density ratio (ρ/ρ_∞) field compared to the results from Palharini (2014) for the tridimensional dsmcFoam simulation of one fourth of the Mars Pathfinder (Palharini, 2014). Figure 4 shows the comparison from experimental density flowfield and from DAC (DSMC Analysis Code) simulations, developed at the NASA Johnson Space Flight Center, as presented by in Allegre et al (1997). According to Allegre (1997) the flowfield density measurement accuracy is estimated to be 10% except for the region encompassing the shock wave located in the forebody region, which is characterized by high-density gradients. Good agreement of density ratio field contours was achieved between the codes.

Figure 5 shows the pressure coefficient (C_p) and Figure 6, the heat transfer flux (q) of the axisymmetric dsmcFoamPlus simulation compared with the DAC, tridimensional dsmcFoam and SR3 experiments. The agreement is very good in the region of the forebody, base plane and sting. However, the same level of agreement is not observed between the present simulated data and the experimental results within the flow expansion on the probe shoulder, where there are no thermocouples located.

Table 3. Drag coefficient for SR3 experiments (Allegre et al, 1997), DAC (Moss et al, 1993), tridimensional dsmcFoam (Palharini, 2014) and axisymmetric dsmcFoamPlus simulation.

	experimental	DAC	dsmcFoam	dsmcFoamPlus
C_D	1.657	1.690	1.652	1.673
$\Delta C_D/C_{D,exp}$	$-$	1.99%	0.30%	0.97%

Table 4. Comparison between axisymmetric dsmcFoamPlus and 3D dsmcFoam simulation parameters (Palharini, 2014).

	# of Cells	Molecules per cell	Molecules simulated
dsmcFoam tridimensional	7125852	10.5	74821446
dsmcFoamPlus axisymmetric	29352	20	587040

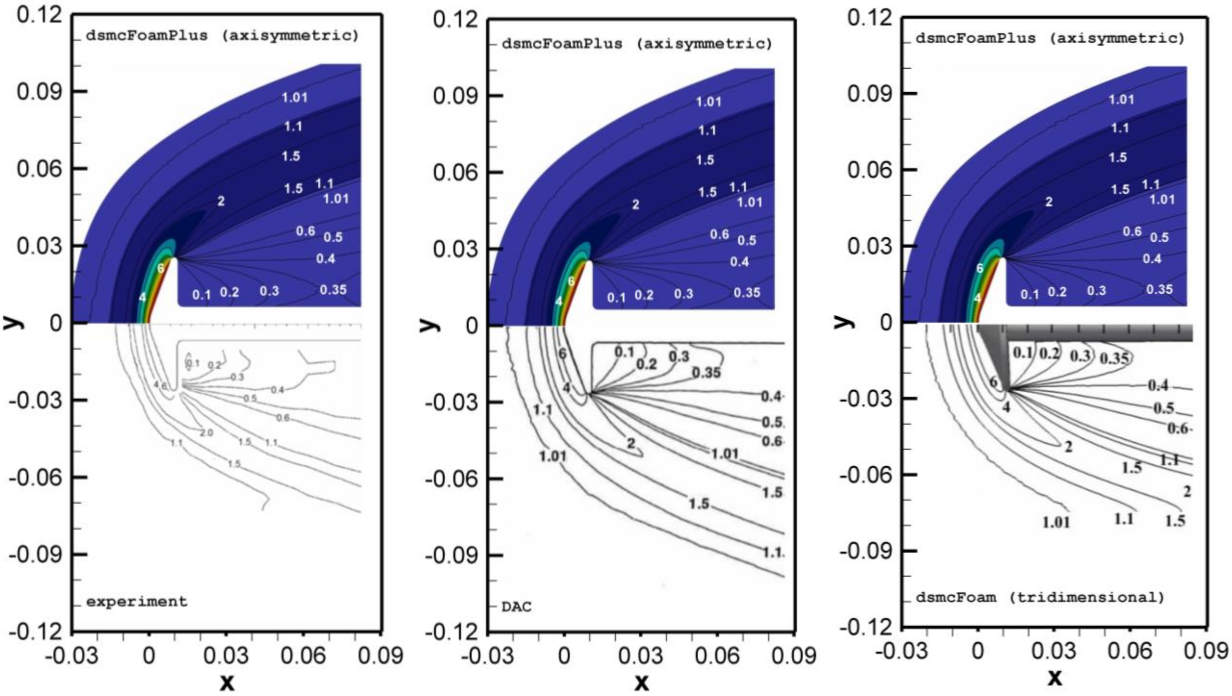

Figure 4. Density ratio (ρ/ρ_∞) distribution for axisymmetric dsmcFoamPlus simulation compared to (a) SR3 experiments (Allegre et al, 1997), (b) DAC (Moss et al, 1993) and (c) tridimensional dsmcFoam (Palharini, 2014).

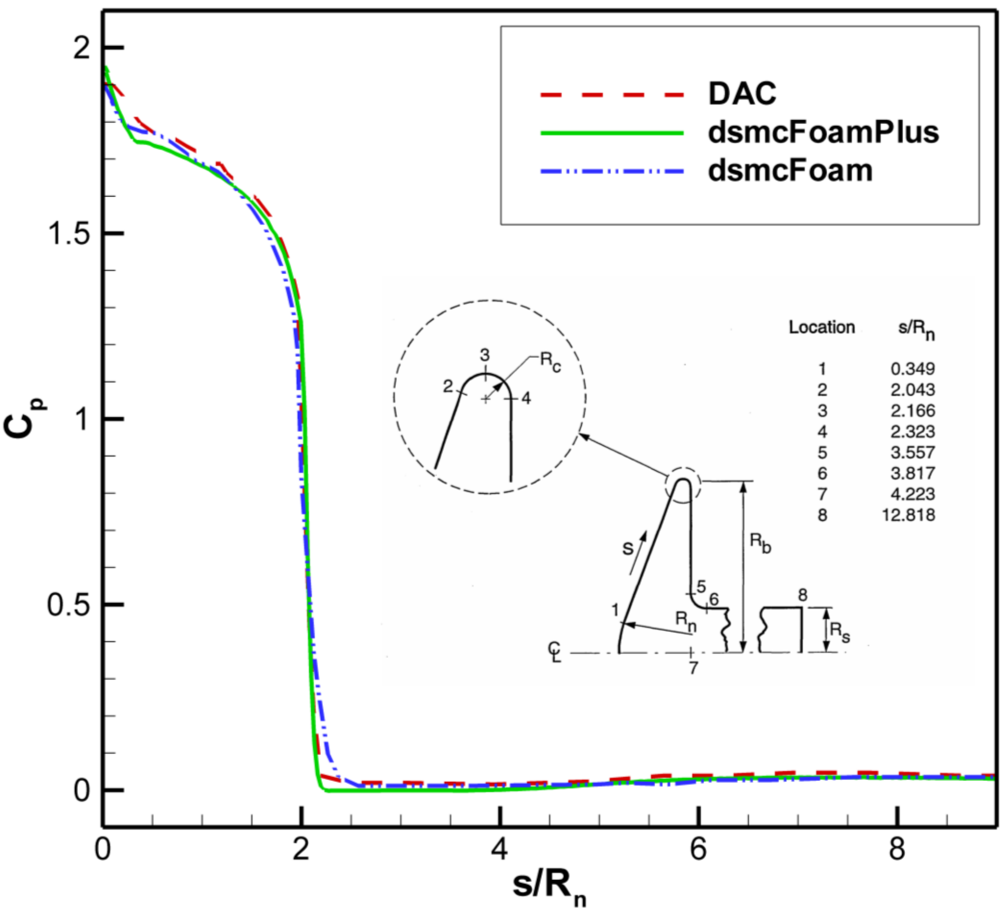

Figure 5. Surface pressure coefficient (C_p) for DAC (Moss et al, 1993), present simulation using axisymmetric dsmcFoamPlus and tridimensional dsmcFoam (Palharini, 2014).

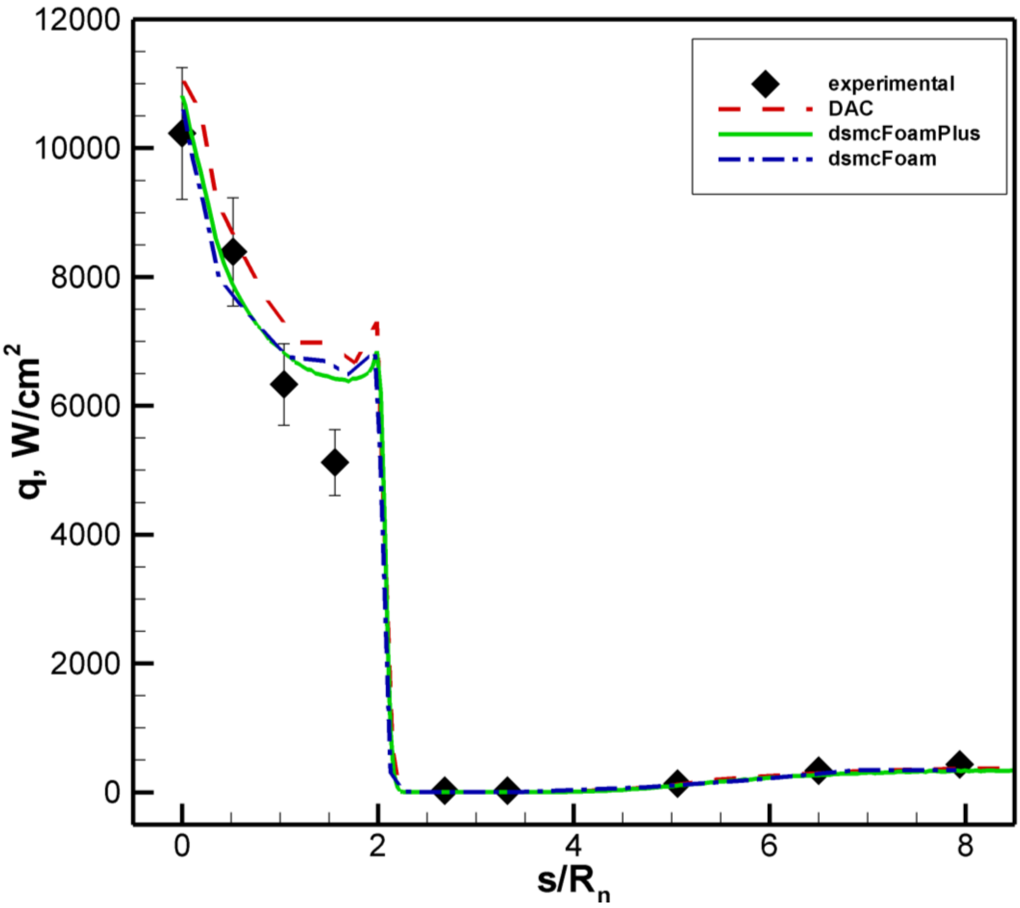

Figure 6. Heat transfer (q) for SR3 experiments (Allegre et al, 1997), DAC (Moss et al, 1993), tridimensional dsmcFoam (Palharini, 2014) and axisymmetric dsmcFoamPlus simulation.

Table 3 shows a comparison between the drag coefficient obtained by experiments and by different DSMC codes. The axisymmetric results show great agreement with an error of less than 1%. Table 4 shows a comparison of the parameters simulated between axisymmetric and tridimensional dsmcFoam implementations. It is possible to see that using a mesh with $7125852/29352 \cong 242$ times less cells and using $74821446/587040 \cong 127$ times less DSMC molecules the results obtained are similar, showing the advantages of using an axisymmetric mesh instead of a tridimensional one.

5. CONCLUSION

Axisymmetric simulation results using the DSMC method were obtained for the hypersonic flow over a 70° blunted cone with the OpenFOAM tool, dsmcFoamPlus. The main goal was the validation of the axisymmetric DSMC code by comparison with the tridimensional dsmcFoam and experimental results.According to this computational work, it is evident that the degree of rarefaction can influence in the strength of the temperature gradients between stagnation and wake regions that should be considered in their thermal protection system design.

It is important to take account the rarefaction effects for high Knudsen number flows, namely, with diffuse shock waves, that influences the calculation of properties in the vehicle wall. In order to accurately predict the reentry of aerospace vehicles, the rarefaction impact on small heat flux predictions in the stagnation point must be taken into account in the aerothermodynamics loads at the design phase.

Furthermore, good agreement was observed when axisymmetric results were compared to wind tunnel experimental data available, showing that the axisymmetric dsmcFoamPlus is an viable tool, in view of giving a computational speed up of a hundred and twenty-seven times, on average, when compared to the three dimensional computations.

6. ACKNOWLEDGEMENTS

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