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# NUMERICAL SIMULATION OF NITROGEN NOZZLE EXPANSION USING KINETIC AND CONTINUUM APPROACHES

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## ABSTRACT

Attitude control of satellites is often accomplished by expanding a gas through the nozzle of small thrusters. The very low background pressure leads to a heavily underexpanded plume, which may impinge on the surrounding surfaces causing contamination, thermal loads and unwanted forces. A thorough understanding of the plume expansion is thus of high importance for the design of a spacecraft and its mission and numerical support of experimental investigations is needed. In a first step towards the development of an efficient numerical methodology that allows for simulation of gas flows over a wide density range, a detached downstream coupling approach of a continuum solver (applicable in regions of high density) and a kinetic particle solver (efficient in regions of low density) has been applied to the problem of nitrogen gas expanding through a nozzle into vacuum. It was found that the approach followed is not sufficient in the investigated flow scenario, as it produces a density discontinuity across large parts of the coupling interface. The reasons for failure of this approach are discussed. The numerical results in the highly rarefied far field of the flow do however agree well with experimental findings.

## 1 INTRODUCTION

For the design and operation of a thruster-controlled spacecraft it is highly desirable to accurately predict the properties of a thruster firing into a vacuum (i.e. space) environment and its interactions with adjacent surfaces. The numerical treatment of such a rapidly expanding flow is however not straight forward. The common methods of Computational Fluid Dynamics (CFD) implicitly assume the gas to be sufficiently dense and at least near a thermodynamic equilibrium, the gas is approximated as continuous matter. This continuum assumption fails however when the average distance between molecules becomes larger. In this case of rarefied gas flow kinetic methods need to be applied to determine the thermodynamic state. Kinetic methods take into account the microscopic, i.e. particulate character of the streaming medium. These methods then inherently allow for non-equilibrium effects to be accounted for, but become computationally expensive in regions of higher density. Thus it seems natural to combine the two numerical approaches and use each where applicable and economic.

There are several attempts documented in the literature to numerically couple continuum and kinetic flow solvers for different applications, with varying degree of complexity and success. However, there seems to be no definite and universal method and there is still considerable ongoing research in this field.

In order to numerically support and complement the experimental investigation of thruster plumes in the high-vacuum test facilities at the Spacecraft Section of the Institute of Aerodynamics and Flow Technology in the German Aerospace Center (DLR), possible ways of combining the DLR's own continuum flow solver TAU [1] with a particle method [2] are to be investigated. To this aim, a well documented reference case of pure nitrogen gas expanding through a conical thruster nozzle into high vacuum is selected to be numerically reproduced and compared to measurements.

To obtain a solution of the whole nozzle flowfield, the efficiency of the continuum solver is to be exploited where applicable, supplying the boundary conditions for the kinetic solver. The hypersonic character of the flow suggests to attempt a pure downstream (i.e. one-way) coupling. The validity of this approach is to be verified.

In the next section the general features of a thruster plume expanding into a vacuum environment are reviewed, before the two numerical methods employed in this work are briefly discussed in section 3. The actual reference case under investigation is presented in section 4. Results are given in section 5, while section 6 summarizes the main
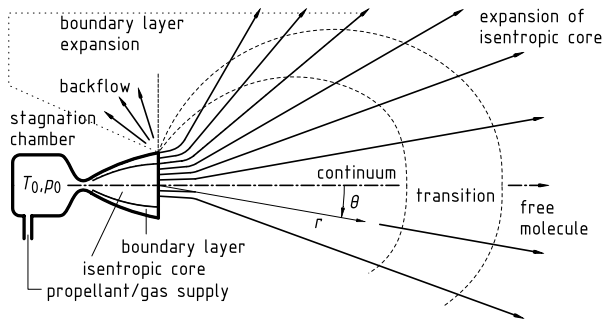
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Figure 1: Schematic view of a nozzle flow expanding into vacuum

aspects of this work and draws conclusions.

## 2   NOZZLE EXPANSION

Gas flow expanding from a reservoir into a high vacuum is characterized by a hypersonic, all-side radial expansion from the exit plane. Figure 1 schematically shows the main features of such a flow.

The gas is assumed to be nearly at rest at the nozzle reservoir, its density is determined by the total pressure $p_0$ and temperature $T_0$. The large pressure gradient causes the gas to accelerate through the nozzle throat, where it reaches sound speed, and subsequently expands as a supersonic flow. In the course of the expansion both density and temperature drop dramatically to adopt to the low background pressure. The decrease in density also decreases the number of intermolecular collisions, thus hindering instant energy exchange among the molecules, leading to thermodynamic non-equilibrium. Both the rarefaction and the subsequent establishment of non-equilibrium lead to a breakdown of the continuum assumption as the gas continues to expand.

When the reservoir temperature $T_0$ is less than or similar to the wall temperature of the nozzle, the expanding and hence cooling flow is effectively heated by the walls in the divergent part of the nozzle. This heating leads to the formation of thick boundary layers with strong gradients that may again be responsible for the formation of thermodynamic non-equilibrium, and thus are subject to treatment by a kinetic approach.

## 3   NUMERICAL METHODS AND PROBLEM APPROACH

### 3.1   Continuum Domain

The methods of classical Computational Fluid Dynamics (CFD) solve a discretized set of partial differential equations, known as the Navier-Stokes equations. These are expressions for the conservation of mass, momentum and energy in a small spatial fluid element and can be derived macroscopically by assuming the gas to be sufficiently dense to be approximated as a continuum, or microscopically by assuming only slight deviation from local thermodynamic equilibrium. If either assumption fails, other, more general descriptions need to be resorted to.

The Navier-Stokes solver used in this work is the DLR TAU code, an implementation of the finite volume method to solve the conservation equations [1].

### 3.2   Rarefied Domain

The numerical simulation of rarefied and strongly non-equilibrium flows require methods that recognize the particulate nature of the gas. As the number of molecules in a reasonably sized macroscopic volume is far too large to simulate their flight and collisions directly even in highly rarefied regimes, one needs to employ statistical methods to characterize the flow. The theoretical framework for these descriptions is layed out by the Kinetic Theory of Gases.

The most efficient, robust and most popular numerical method today for treating rarefied gas flows is called Direct Simulation Monte Carlo (DSMC) [3]. The algorithm employs simulator molecules, each representing a large ensemble of real particles, and decouples their motion and collisions within a timestep: first, the position of the particles is updated according to their velocities, regardless of wether the trajectories might intersect. Then collisions between nearby molecules are carried out on a stochastical basis. To obtain macroscopic quantities like density, bulk velocity and temperature, the properties of the particles are sampled over many timesteps. The actual number of timesteps used for sampling determines the amount of statistical scatter in the solution.

As physically accurate simulations rely on a spatial resolution of the order of a particle's mean free path (i. e. the average distance between two subsequent intermolecular collisions) and a meaningful number of particles within a cell is required to

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keep statistical scatter low, the DSMC method gets computationally more expensive as the gas density increases. It is thus limited by economic, not by physical constraints.

## 3.3 Determination of Interface Conditions

The two fundamental questions associated with combining two simulation methods is *where* to couple them and *how* the coupling is to be done. In this work the codes are to be combined along a physically significant boundary, and hence the first question associated with the location of the flow interface requires the definition of a criterium that signals the domain of validity for the CFD method.

The number of concurrently employed continuum breakdown parameters in recent literature suggests difficulties in singling out one universally applicable criterium and several proposed formulations have been trialed in the course of this work.

A well known non-dimensional parameter characterising the degree of rarefaction in a flow is the so-called Knudsen number Kn, relating the mean free path $\lambda$ to a characteristic dimension of the flow. To avoid arbitrariness in the definition of a characteristic flow length, it is frequently suggested to employ a gradient length based on a flow parameter $Q$, such as density $\rho$, speed $u$ or temperature $T$ [4]:

$$\mathrm{Kn_Q} = \lambda \frac{|\nabla Q|}{Q}, \qquad Q \in \{\rho, u, T\}. \qquad (1)$$

These can be shown to be not completely independent of each other, and the Knudsen number based on density is most frequently used.

The Navier-Stokes equations of continuum gas dynamics can be derived from kinetic theory by assuming only small deviation from local thermal equilibrium. This small deviation introduces terms associated with heat flux $\boldsymbol{q}$ and shear stress $\boldsymbol{\tau}$. It is thus reasonable to assume, that the magnitude of these non-equilibrium terms may indicate the degree of deviation from local thermal equilibrium. One such parameter has been put forth by Garcia et al. [5], it simply compares the suitably normalized values of the non-dimensional heat flux and shear stress:

$$B = \max(|\hat{\boldsymbol{q}}|, |\hat{\boldsymbol{\tau}}|). \qquad (2)$$

The parameter $B$ can be shown to slightly overpredict continuum breakdown if compared to more rigourous mathematical derivations, and thus lends itself well as a breakdown parameter.

Of the different breakdown criteria investigated in this work, the Knudsen number based on the
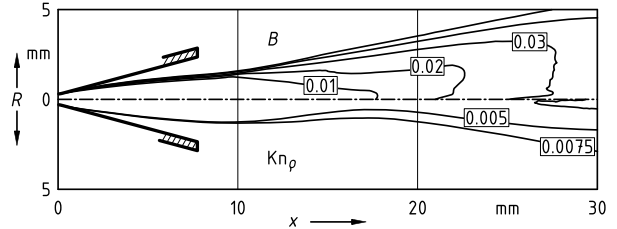


Figure 2: Comparison of continuum breakdown in the flow investigated here (see section 4) predicted by the Knudsen number based on the density gradient (bottom) and parameter $B$ based on non-equilibrium terms in the Navier-Stokes equations

density gradient lenght, $\mathrm{Kn}_\rho$, and the parameter $B$ seemed most promising to detect the continuum limit where it would be expected from experimental observations. Figure 2 compares $\mathrm{Kn}_\rho$ and $B$ when applied to the flow under investigation in this work. Two important conclusions can be drawn from Figure 2: first, both parameters (and in fact all others investigated) clearly signal non-equilibrium in the thick boundary layer, up to the nozzle throat. Second, the anticipated pear-shaped structure of the continuum domain (cf. Figure 1) is only reproduced by parameter $B$[1]. The suggestions for an actual limiting value for all breakdown parameters vary greatly and separate investigations carried out in the course of this work indicated that a value around $B = 0.03$ would result in an acceptable trade-off between best-possible physical accuracy and a smallest possible DSMC domain.

The second question posed at the beginning of this subsection was concerned with how to couple the two solvers along the interface detected by the continuum breakdown parameter. As a two-way communication between a DSMC solver and a classical CFD code poses significant challenges due to the scatter inherent in results of the DSMC simulation, it was decided to follow a most simple approach: The whole flowfield is initially computed with the CFD solver with as low a background density as possible and disregarding physical appropriateness. Then a continuum breakdown parameter is applied to the solution and a coupling interface is determined. This interface line acts as an inflow boundary for the DSMC domain and the boundary conditions (density, velocity, temperature) are extracted from the CFD solution. This essentially

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[1]The unphysical shape of the contour lines near the nozzle axis is due to occasional difficulties with gradient reconstruction in axisymmetric simulations
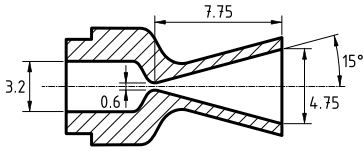
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Figure 3: Geometric dimensions of the DASA 0.5N conical nozzle (values given in mm)

corresponds to a one-way transport of information from the CFD into the DSMC domain, labeled "downstream coupling" in this text. It is expected that this simplification is justifiable in the case of hypersonic nozzle flows since supersonic flows are indeed characterised by carrying information only downstream, and typically there is only one interface between the continuum and the rarefied domain, as illustrated in Figure 1.

## 4 REFERENCE CASE

### 4.1 Nozzle Geometry

To allow for direct comparison of numerically obtained results with experimental measurements, a small conical thruster nozzle is selected for which there are numerous experimental results available. The geometry of the nozzle is displayed in Figure 3. Note, that it is actually quite small, with an exit diameter of slightly less than 5 mm and a throat diameter of 0.6 mm. When used in a real thruster configuration with hydrazine as originally designed, it produces a nominal thrust of about 0.5 N.

### 4.2 Boundary conditions

In experimental investigations of nozzle plume characteristics it is sometimes desirable to reduce the complexity of the flow and to be able to have better control of the conditions in the nozzle reservoir. Therefore, many experiments are carried out with so-called "simulated plumes" of a pure gas. As nitrogen is the primary constituent of decomposed hydrazine and also readily available in pressurized containers, nitrogen is frequently used as a test gas for experimental investigations.

One of the best documented sets of data for the nozzle under investigation is available at DLR for reservoir pressure $p_0 = 0.5$ bar and reservoir temperature $T_0 = 300$ K. The nozzle wall may be approximated as isothermal at a temperature of $T_W = 300$ K.

The experimental data was obtained in the DLR High-Vacuum Plume Test Facility (STG) [6], which is a large cryo-pumped vacuum chamber of about

$10\,\mathrm{m}^3$ expansion volume that is capable of maintaining a background pressure of $p_b < 10^{-8}$ bar while the thruster is in operation. This space-like condition can be kept up because the walls of the cryo pump are cooled with liquid helium at a temperature of about 4 K, and the molecules hitting the wall simply freeze out.

The walls of the vacuum chamber are however not accounted for in the numerical simulation and a so-called vacuum boundary is assumed, that is, particles are only leaving the computational domain across this boundary.

As described in section 3, the whole flowfield is initially computed with the continuum solver, which requires boundary conditions to be specified at the farfield outflow boundaries. A minimum density in the order of $\rho_\infty \approx 10^{-7}\,\mathrm{kg/m}^3$ could be applied before the solver experienced stability problems. Together with a temperature of about $T_\infty \approx 10$ K this results in a pressure of the same order of magnitude as can be attained by the cryo pump.

The DSMC inflow boundary conditions $\rho$, $u$ and $T$ are extracted from the CFD solution along the interface line determined by the continuum breakdown parameter (see subsection 3.3).

## 5 RESULTS

Two aspects need to be verified to judge the applicability of the pursued detached downstream coupling approach. One is concerned with the vicinity of the coupling interface (near field), which needs to exhibit physically reasonable (i.e. smooth) state transition from the continuum to the kinetic domain, the other is of more pragmatic nature, namely to determine how well the numerical results can reproduce the experimental data in the far field.

### 5.1 Near Field Results

A successful coupling of two solvers along an interface is characterized by not displaying discontinuities of flow variables across the interface. Figure 4 shows plots of normalized number density $n$ and temperature $T$ in two representative planes A and B perpendicular to the coupling interface. The location of A and B is clarified in the inset: A intersects the interface at the nozzle exit, while B is located at the downstream end of the continuum domain, just off the nozzle axis.

In observing the trends of $n$ and $T$ it immediately becomes apparent that the temperature transitions smoothly from one domain into the other, while the
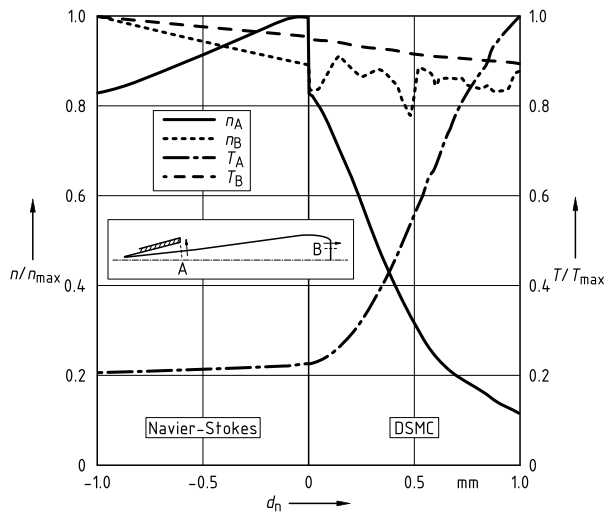
Figure 4: Comparison of density ($n$) and temperature ($T$) variation across the coupling interface in two locations, A and B



Figure 5: Connection of the molecular Mach number normal to the coupling interface, $S_n$, to the ratio of particles entering/leaving the DSMC domain, $N_+/N_-$

number density shows unnatural behavior in both planes. These deficiencies need discussion. Obviously, in plane A the density in the DSMC domain is just over 80% of the value at the continuum side of the coupling interface, which may seems surprising at first, as the continuum value of the density is directly prescribed as a boundary condition for the DSMC solver.

To understand this effect, one needs to recall that DSMC is treating the flow as composed of a large number of particles, each having a random thermal velocity component superimposed on the macroscopic, observable bulk flow velocity. A non-dimensional parameter commonly applied to characterize a flow of molecules is the molecular Mach number $S$, which is defined in analogy to the Mach number of gas dynamics, but relating the flow speed $u$ to the most probable thermal speed $\tilde{c}$ of the random molecular motion:

$$S = \frac{u}{\tilde{c}}. \tag{3}$$

This description can be applied to a flow crossing an interface, by simply defining a local molecular Mach number $S_n$ perpendicular (normal) to the interface, thereby comparing the perpendicular velocity component $u_n$ to the most probable thermal speed.

If the normal component of th flow velocity is in the order of the most probable thermal speed or smaller, i.e. if $S_n \lesssim 1$, a significant number of molecules (namely the ones with a high negative thermal velocity component) actually cross the interface in the opposite direction of $u_n$.
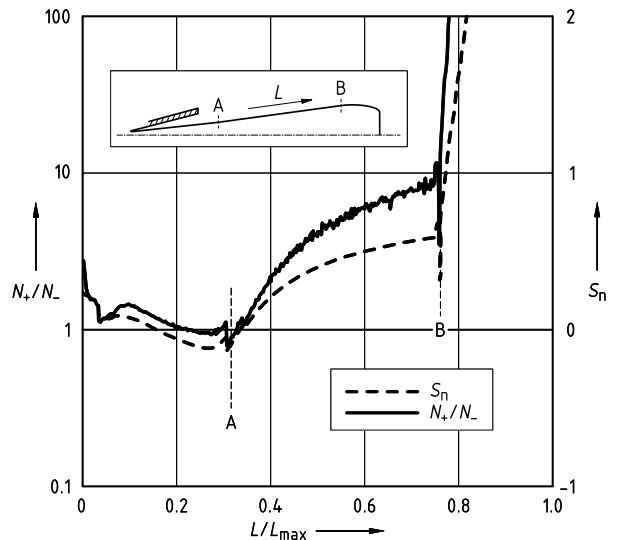
The coupling interface was chosen in this work on a purely physical basis and it was stated in subsection 3.3, that large gradients in the boundary layer caused breakdown of the continuum assumption in the shear layer between the near-isentropic core of the nozzle flow and the boundary layer. The interface thus determined on physical reasoning is however nearly parallel to the flow streamlines for the most part of the identified continuum limit, and hence the normal component of the velocity is mostly very small.

Figure 5 attempts to visualize this problem. The inset again shows the inflow boundary of the DSMC domain, in this figure A and B are two points placed on the interface line to assist the readability of the graph. The dash-dotted line shows the normal molecular Mach number $S_n$ (right ordinate) along the relative length $L$ of the coupling interface. For comparison, the solid line referring to the left ordinate is an actual recording of the ratio $N_+/N_-$ of particles entering, respectively leaving the DSMC domain during the simulation. Clearly these curves are connected. Note, that along 80% of the DSMC inflow boundary a significant fraction of particles are leaving the kinetic domain towards the continuum domain. As the information carried by these molecules is not accounted for in a downstream coupling approach, the conditions at the interface must be erroneous and the most obvious effect was seen in the density profile at plane A in Figure 4.

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The large fluctuations observed in the density profile at plane B in Figure 4 is however not due to the coupling approach, since the normal molecular Mach number in the donstream region of the continuum domain is sufficiently large (cf. Fig. 5). The scatter seen here is a problem inherent in axisymmetric DSMC simulations as only very few particles can be relied on for sampling the flow variables near the axis. This deficiency may be overcome by suitably modifying the underlying algorithm [3], but this was beyond the scope of this work. The general trend of the density decrease across the interface at plane B in Figure 4 can however be observed.

## 5.2 Far Field Results

It is interesting to observe how the unsatisfactory results in the nearfield of the nozzle will affect the numerically determined flow field variables further away from the coupling interface.

A standard experimental technique employs a so-called Patterson probe to determine the particle flux (net number of particles crossing a unit area in unit time) in highly rarefied gases. Particle flux measurements at various positions in the flowfield for the setup investigated here were already available as angular and radial profiles at distance $r$ measured from the nozzle exit plane and angle $\theta$ measured from the axis of symmetry. A representative angular profile at $r = 0.5\,\text{m}$ comparing the measured values of particle flux (crosses) and the results of the DSMC calculation (solid line) is displayed in Figure 6.

Despite the problems at the DSMC inflow boundary, discussed in the previous subsection, the far field results agree quite well. There are two discrepancies to be noted and discussed, the most obvious being the "dent" in the numerical results at $\theta = 0°$. This unphysical result has to be attributed to general problems of less sophisticated axisymmetric DSMC procedures near the axis of symmetry. Apart from that the measurements yield a noticeably higher particle flux in the region of $45° < |\theta| < 90°$. This may be explained by again resorting to a description of the gas at a molecular level. For simplicity, the nozzle wall was assumed to be of uniform temperature in the simulation, while in reality it will be cooler at the nozzle lip than near the nozzle throat. Since particles colliding with the wall are assumed to be reemitted diffusively, i.e. assuming a random thermal velocity depending on the wall temperature, a warmer wall will result in a more pronounced thermal motion, which in turn leads to a larger number of particles in the back
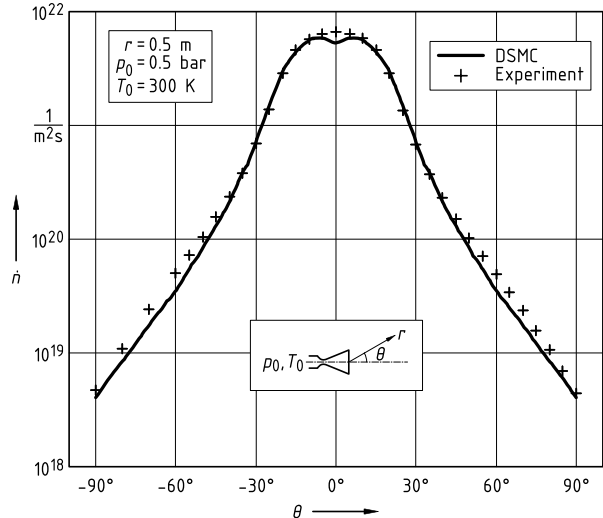


Figure 6: Angular profile of particle flux $\dot{n}$ at $r = 500\,\text{mm}$ from the nozzle exit plane, comparison of experimental results and numerical simulation

flow ($\theta > 90°$) and a smaller fraction of molecules reaching areas further downstream. Also the observed lower density in the boundary layer due to the suboptimal coupling conditions may contribute to the lower particle flux.

In Figure 7 radial profiles of particle flux at different constant angles $\theta$ are compared with the available experimental data. One immediately recognizes the steady divergence of measurements and numerical results in this double logarithmic plot for $\theta = 90°$. These differences are however certainly not due to deficiencies in the simulation, as the results for $r = 500\,\text{mm}, \theta = 90°$ agreed well in the angular profile, and the numerically obtained results successfully and correctly reproduce the theoretically predicted and previously observed inverse quadratic dependence of particle flux on $r$.

## 6 SUMMARY AND CONCLUSION

In a first step towards the development of a numerical method that allows for simulation of gas flows over a wide density range, a detached downstream coupling approach of a continuum solver and a kinetic (particle) solver has been applied to the problem of a gas expanding through a nozzle into vacuum. Hybrid continuum/kinetic solvers are necessary to allow for an efficient numerical simulation of a wide density range of flows as they particularly appear in space technology.

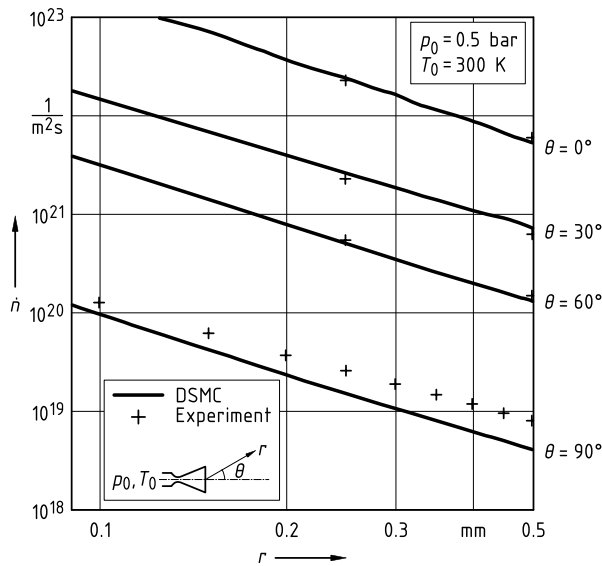The particular case of a nozzle flow expanding

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Figure 7: Radial profiles of particle flux $\dot{n}$ at varying angles, distance $r$ measured from nozzle exit plane

into vacuum is closely related to the study of the unwanted impingement effects induced by a thruster firing into a space environment. Because of the low background pressure, the plume will expand radially in all directions, impinging on adjacent surfaces and thus causing contamination, thermal loads and forces that are difficult or impossible to estimate. In the work described in the previous sections, the focus was on obtaining a numerically efficient solution of the expanding flow field with as little effort as possible. Interactions with surfaces was not part of this investigation and the flow field was assumed to be axisymmetric.

The flow field was calculated in a serial fashion by determining an initial solution using only a continuum solver, which will necessarily deliver incorrect results in areas where the continuum assumption fails. The validity limit was determined via suitable continuum breakdown indicators. Large gradients in the shear layer cause these breakdown parameters to signal non-equilibrium in the whole (thick) boundary layer, up to the nozzle throat. More than 80% of the coupling interface is thus nearly parallel to the flow direction. In a molecular picture, this means significant backflow of particles into the continuum domain, hence the assumption of uni-directional transport of information is violated, which becomes manifest in an unphysical density jump across the coupling interface. A pure downstream coupling is thus not applicable to this kind

of flow and more sophisticated procedures need to be developed.

The failure to reproduce a continuous transition of flow variables across the coupling interface however appears not to have a significant impact on the flowfield far downstream of the nozzle exit plane. The numerical results agree quite well with experimental findings.

The development of hybrid continuum/DSMC methods remains an active field of research, since (upstream) coupling to Navier-Stokes solvers poses difficulties mostly due to the stochastical nature of the employed DSMC algorithm. A flexible 3D, state-of-the-art DSMC solver is currently developed, bearing in mind possible coupling approaches to the DLR TAU code to allow for a numerical treatment of flow interaction with realistic spacecraft geometries.

## Acknowledgements

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