Numerical Simulation of Nozzle Flow into High Vacuum Using Kinetic and Continuum Approaches

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Summary

Laminar nitrogen flow expanding through a conical nozzle into high vacuum is to be numerically reproduced and compared to available experimental data. As the gas density varies quickly by several orders of magnitude, leading to high rarefaction and thermal non-equilibrium, standard (continuum) CFD tools are not sufficient to accurately model the expanding flow. In the work presented here, the efficiency of Navier-Stokes solvers is to be exploited where applicable, supplying the boundary conditions for a kinetic Direct Simulation Monte Carlo (DSMC) solver to handle the domain of rarefaction and non-equilibrium. The hypersonic character of the flow suggests to attempt a pure downstream coupling. The validity of this approach is to be verified.

1 Introduction

The experimental investigation of small satellite thruster plumes is an important area of research in the Spacecraft Section of the DLR Institute of Aerodynamics and Flow Technology and the unique DLR High-Vacuum Plume Test Facility (STG) allows for investigation of plume expansion under space-like conditions. STG is a large cryo-pumped vacuum chamber of about $10\,\mathrm{m}^3$ expansion volume that is capable of maintaining a background pressure of $p_\mathrm{b} < 10^{-8}$ bar while the thruster is in operation. Suitable numerical methods to support the experiments are however not readily available, as the common Navier-Stokes solvers may only be applied to the dense, near-isentropic core of the flow, while the non-equilibrium regime of the plume expansion has to be treated by kinetic methods such as Direct Simulation Monte Carlo (DSMC). Solving the whole of the nozzle flow with the DSMC method is however prohibitively inefficient.

In order to support and complement the experimental investigation of thruster plumes in the STG, 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 flow field, 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 coupling. The validity of this approach is to be verified.

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 at a pressure p_0 and temperature T_0. The rapid expansion downstream the nozzle throat and hence the decrease in density also decreases the number of intermolecular collisions, thus hindering instant energy exchange among the molecules and leading to thermal non-equilibrium. The rarefaction and the subsequent establishment of non-equilibrium lead to a breakdown of the continuum assumption as the gas continues to expand.

When T_0 is of similar order or less than the temperature of the nozzle wall, the effective flow heating leads to the formation of thick boundary layers with strong gradients that may again be responsible for the formation of thermal non-equilibrium, and thus are subject to treatment by a kinetic approach.

3 Numerical Methods and Problem Approach

It is well known that the conservation equations of mass, momentum and energy in a small spatial fluid element can be derived macroscopically by assuming the gas to be sufficiently dense to be approximated as a continuum, or microscopically from the Boltzmann equation by allowing only a small deviation from local thermal equilibrium. This implies that typical lenght- and time scales of a particular problem are large compared to the molecular mean free path or mean time between intermolecular collisions. If either assumption fails, more general descriptions need to be resorted to.

The tool used in this work to treat this so-called continuum domain is the DLR TAU code, an implementation of the finite volume method to solve the conservation equations [1].

The numerical treatment of rarefied and strongly non-equilibrium flows require methods that recognize the particulate nature of the gas. The most efficient, robust and most popular numerical method today for treating rarefied gas flows is termed 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 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.

3.1 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 criterion 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 criterion and several proposed formulations have been trialed in the course of this work.

A well known parameter characterizing the degree of rarefaction in a flow is the Knudsen number Kn, relating the mean free path λ to a characteristic dimension. It is frequently suggested to employ a gradient length based on some flow parameter Q, such as density ρ, speed u or temperature T [4]:

$$\mathrm{Kn_Q} = \lambda \frac{|\nabla Q|}{Q}, \text{ where } Q \in \{\rho, u, T\} \quad . \tag{1}$$

These can be shown to be not 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 q and shear stress τ. 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 compares the suitably normalized values of the non-dimensional heat flux and shear stress:

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

The parameter B can be shown to slightly over-predict 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 density gradient lenght, Kn_ρ, and the parameter B seemed most promising to detect the continuum limit where it would be expected from experimental observations. Figure 2 compares Kn_ρ and B when applied to the flow under investigation in this work. Two important conclusions can be drawn from Fig. 2: first, both parameters (and in fact all others investigated) clearly signal non-equilibrium in the boundary layer, up to the nozzle throat. Second, the anticipated pear-shaped structure of the continuum domain (cf. Fig. 1) is only reproduced by parameter B. 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 flow field 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 corresponding boundary conditions are extracted from the CFD solution. This essentially 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 flows.

4 Reference Case

A small conical thruster nozzle (cf. Fig. 3) is selected for which there are numerous experimental results available [6]. One of the best documented sets of data for the nozzle under investigation is available at DLR for pure nitrogen flow at $p_0 = 0.5\,\mathrm{bar}$ and $T_0 = 300\,\mathrm{K}$. The nozzle wall may be approximated as isothermal at a temperature of $T_W = 300\,\mathrm{K}$.

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. It immediately becomes apparent that the temperature transitions smoothly from one domain into the other, while the number density shows unnatural behavior in both planes. In plane A, the density in the

DSMC domain, right at the coupling interface, is noticeably smaller than the value at the continuum side of the same location. 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. The ratio of the flow speed u to the most probable thermal speed $\tilde{c}$ of the random molecular motion (approximately equal to the sound speed) is called molecular Mach number S. If the normal component of the flow velocity is in the order of the most probable thermal speed or smaller, i. e. if $S_{\mathrm{n}} \lesssim 1$, a significant number of molecules 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 3.1, 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. This explains the discontinuity of the density profile A in Fig. 4. Though density profile B exhibits large amplitudes of scatter, which is a well known problem in axisymmetric DSMC simulations, the general trend does not indicate a density jump. This is expected, as S_{n} is much greater than one at this position of the interface.

5.2 Far Field Results

Particle flux measurements at various positions in the flow field for the setup investigated here were already available as angular and radial profiles at distance r measured from the nozzle exit plane and angle θ measured from the axis of symmetry. A representative angular profile at $r = 0.5\,\mathrm{m}$ comparing the measured values of particle flux (crosses) and the results of the DSMC calculation (solid line) is displayed in Figure 5.

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, the most obvious being the "dent" in the numerical results at $\theta = 0^{\mathrm{o}}$. 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 $45^{\mathrm{o}} < |\theta| < 90^{\mathrm{o}}$. 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 flow ($\theta > 90^{\mathrm{o}}$) 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.

6 Conclusion

Large gradients in the shear layer cause the continuum 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. This deficiency however appears not to have a significant impact on the flowfield far downstream of the nozzle exit plane. The downstream coupling approach may thus be sufficient for an engineering estimation of flow field conditions distant from the nozzle.

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.

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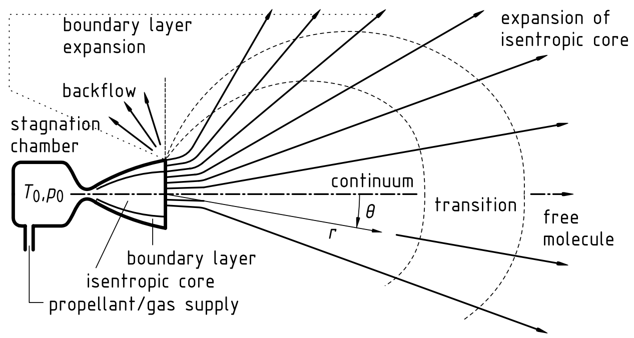

Figure 1 Schematic view of a nozzle flow expanding into vacuum

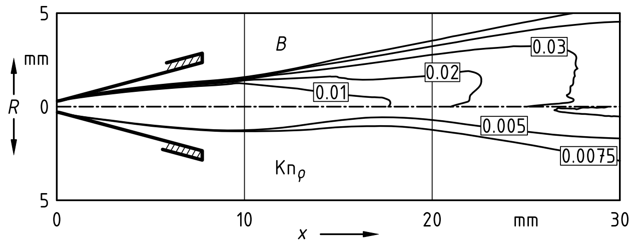

Figure 2 Comparison of continuum breakdown in the flow investigated here (see Sec. 4) predicted by the Knudsen number based on the density gradient (bottom) and parameter *B* based on non-equilibrium terms in the Navier-Stokes equations

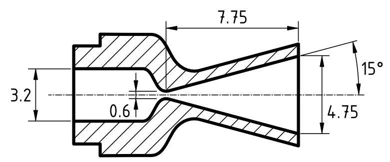

Figure 3 Geometric dimensions of the DASA 0.5N conical nozzle (values given in mm)

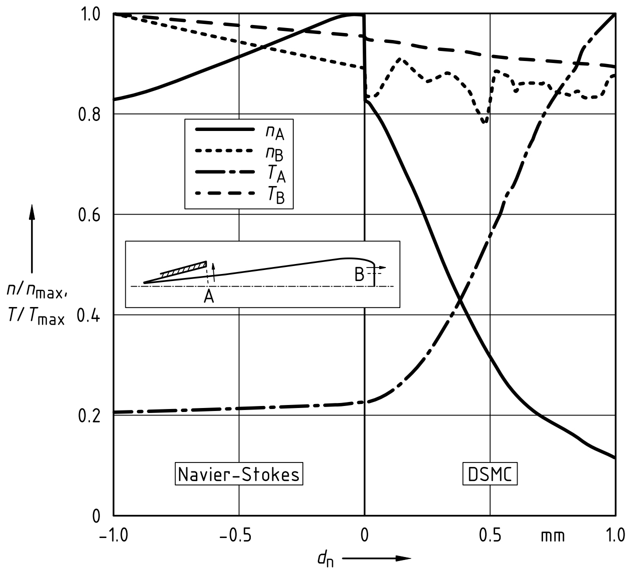

Figure 4 Density (n) and temperature (T) variation across the coupling interface

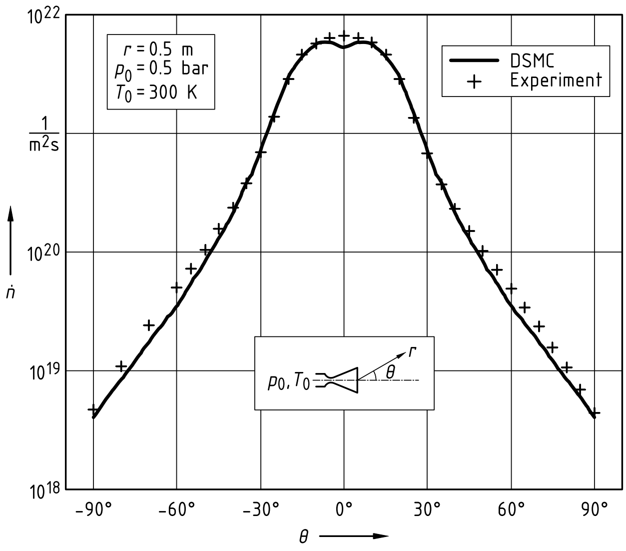

Figure 5 Angular profile of particle flux $\dot{n}$ at $r = 500$ mm from the nozzle exit plane