Numerical Study of Backflow for Nozzle Plumes Expanding into Vacuum

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This work is prompted by recent experiments on a multiphase (gas/droplets/cooling film) flow expanding from a supersonic nozzle into vacuum. A reverse motion of droplets (in the direction opposite to the flow in the plume core) has been experimentally observed near the nozzle lip. To understand this phenomenon, we have performed a numerical investigation of backflow formation. A hybrid Navier-Stokes/Direct Simulation Monte Carlo approach has been used to simulate the flow in different regimes — from a dense flow inside the nozzle, through very fast expansion near the nozzle lip, to a rarefied, free-molecular flow in the backflow region. A Lagrangian particle algorithm has been employed to trace the droplet motion in the gas flow. It has been shown that the gas backflow constitutes only a small part of the total mass flow rate. As a result, aerodynamic forces are insufficient to turn the droplets around the nozzle lip, and it seems that none of the droplets from the nozzle cannot reach the backflow region. Thus, it can be assumed that all droplets in the backflow originate from the cooling film being destroyed on the nozzle lip. Further, to investigate the viscous expansion flow near the nozzle lip in more detail, a model problem — the flow over a plane wall turning by a large angle (an expansion corner), has been studied using both continuum and kinetic modeling. It has been shown that, due to viscous effects, the flow deviates drastically from the classical Prandtl-Meyer solution. For large deflection angles, the decrease in the flow Mach number and the growth of the flow temperature are observed instead of their increase and fall, respectively. Reasons for such behavior are discussed, and the limits of applicability of the Navier-Stokes solution are analyzed.

Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
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<tr>
<td>F</td>
<td>Mass flow rate</td>
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<tr>
<td>M</td>
<td>Mach number</td>
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<tr>
<td>n</td>
<td>Normal-to-wall coordinate, m</td>
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<tr>
<td>p</td>
<td>Pressure, Pa</td>
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<tr>
<td>Pr</td>
<td>Prandtl number</td>
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<tr>
<td>r</td>
<td>Distance from corner vertex</td>
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I. Introduction

It is well known that the spacecraft surface contamination processes may significantly degrade performance of systems exposed to the space environment.\textsuperscript{1} For orbital space stations such as the Russian station Mir or International Space Station, one of the most important sources of contamination is control thruster exhaust products. During thruster firing, a large amount of propellant is exhausted into space, and droplets forming as a result of liquid fuel condensation and breakup of the nozzle cooling film can reach the spacecraft surface. This phenomenon was reproduced in the model experiments\textsuperscript{2–5} with gas-droplet plumes issuing from supersonic nozzles into vacuum chambers. It was observed that, in the vicinity of the nozzle lip, some droplets were moving in directions making angles greater than 90° with the nozzle axis. One of the possible mechanisms provoking the reverse motion of liquid droplets may be the carrier-gas backflow originating from the nozzle boundary layer, which turns sharply around the nozzle lip while undergoing continuum expansion and then passing into transitional and free-molecular regimes as the density decreases. It can be assumed that the gas flow drags the droplets from the nozzle into the backflow region. On the other side, the droplets in the backflow can originate from the breakup of the cooling film on the nozzle lip rather than from the gas/droplet flow in the nozzle itself. In any case, a better understanding of gaseous backflow properties may be of great importance for the problem of spacecraft-surface contamination. It should be noted that, in spite of a number of experimental\textsuperscript{6,7} and numerical\textsuperscript{8–10} studies on backflow formation, this subject is far from being fully understood.

The goal of the present work is a detailed numerical investigation of the backflow formation phenomenon, using a hybrid approach combining the continuum (Navier-Stokes, NS) and kinetic (Direct Simulation Monte-Carlo, DSMC) computations. As a rule, a Navier-Stokes solver is used to simulate a dense flow inside a supersonic convergent/divergent nozzle, while the flow around the nozzle lip and in the backflow region is computed with a DSMC code. To investigate the influence of the Reynolds number, the computations are performed for two different axisymmetric conical nozzles. First, the low-Reynolds-number nozzle flow with a thick boundary layer and only a small inviscid core, which was studied experimentally by Rothe,\textsuperscript{11} is considered. Second, a moderate-Reynolds-number flow corresponding to the conditions of recent experiments\textsuperscript{5,12} at the Institute of Thermophysics (Novosibirsk) is simulated. Further, the flowfields obtained
are utilized in computations of droplet motion using a Lagrangian particle code. Finally, in order to study backflow formation near the nozzle lip in more detail, a model problem is considered, in which the viscous flow expansion over an expansion corner (a plane wall turning suddenly by a large angle) is simulated with both the Navier-Stokes and DSMC codes. The results are compared and analyzed.

The remainder of paper is organized as follows. In Section 2 numerical techniques for solving the Navier-Stokes equations, DSMC simulations, their hybridization, and Lagrangian tracking of droplet motion are briefly described. The results of numerical simulations of nozzle and plume flows are presented in Section 3. In Section 4, the viscous flow over an expansion corner is considered. The conclusions are formulated in Section 5.

II. Numerical approach

A. Navier-Stokes numerical technique

The two-dimensional and axisymmetric Navier-Stokes equations are solved with a shock-capturing MUSCL TVD scheme. The standard van Leer’s formula with the minmod slope limiter is used for reconstruction of cell-faced variables from cell-centered ones. The viscous terms are approximated by the central finite differences and the HLLEM approximate Riemann solver is employed to calculate the inviscid fluxes. The HLLEM solver is constructed to be robust near low densities and, therefore, it is particularly appropriate for simulation of rapidly expanding flows such as in the present paper.

For low-Reynolds-number regimes, the initial rarefaction effects are taken into account by means of imposing velocity slip and temperature jump boundary conditions on solid walls. For this purpose, the slip conditions deduced by Kogan are used:

\[ u_r = 2 - a_u \alpha_u \lambda \frac{\partial u_r}{\partial n}, \quad T - T_w = 2 - a_e \alpha_e \frac{\gamma}{(\gamma - 1) \text{Pr}} \lambda \frac{\partial T}{\partial n}, \quad \lambda = \mu \sqrt{\frac{\pi}{2 \rho}}. \]

(B1) Here \( a_u = 0.858 \) and \( a_e = 0.827 \) are numerical coefficients derived from an approximate solution of the linearized Boltzmann equation in the Knudsen layer near the solid wall. The accommodation coefficients for momentum \( \alpha_u \) and energy \( \alpha_e \) are taken equal to unity because no reliable data are available for their values for the present experimental conditions.

B. DSMC numerical technique

The DSMC code SMILE developed in Computational Aerodynamics Laboratory, Institute of Theoretical and Applied Mechanics is utilized for kinetic modeling. Intermolecular collisions are computed by the Variable Hard Sphere (VHS) model. The number of collisions is calculated by the majorant frequency method. In the case of a polyatomic gas, the energy redistribution between rotational and translational degrees of freedom is obtained in accordance with the Larsen-Borgnakke model with a constant rotational collision number. Up to \( 9.6 \times 10^6 \) molecules are used to simulate the flows under consideration. The computations are performed on a 16-processor Linux cluster.

C. Hybrid algorithm

In the course of hybrid simulations, a coupling of Navier-Stokes solver and the DSMC method is based on the use of the NS solver in the nozzle and in the plume core and the DSMC method in the in the neighborhood of the nozzle lip and in the backflow region. Flow parameters on the boundaries of the DSMC computational domain, which are located inside the nozzle and in the central part of nozzle plume, are taken from a previous Navier-Stokes simulation. The velocity distribution function, which is needed to provide necessary boundary conditions for the DSMC method, is specified as the local Maxwellian distribution. It is worth noting that, from the general viewpoint, the Chapman-Enskog distribution function is a natural choice for model particles coming into the DSMC computational domain at the boundary between the NS and DSMC domains. However, the Chapman-Enskog distribution function has a drawback: it becomes negative with deviation from the Maxwellian distribution. Moreover, it was demonstrated in a number of works (see, e.g.) that the Chapman-Enskog distribution function may not provide much improvements against the Maxwellian distribution. As our simulations also demonstrate, the simplest approach to NS/DSMC coupling based on the local Maxwellian distribution works quite well for the present conditions. An example of the
hybrid simulation for a low-Reynolds-number conical nozzle is shown in Fig. 1. The thick and thinner red lines are the boundaries of computational domains for the continuum and kinetic simulation, respectively. The density contours are shown as solid (for Navier-Stokes) and dashed (for DSMC) curves. From this figure, close agreement between two solutions in the common part of two computational domains is evident.

![Figure 1. An example of the hybrid continuum/kinetic simulation of low-Reynolds-number flow in a conical nozzle.](image)

D. Lagrangian tracking of liquid droplets

The description of liquid droplets is based on the Lagrangian approach, in which the disperse phase is considered as a set of discrete probe particles. Their dynamics is governed by the balance equations for mass, momentum, and internal energy of each particle. These equations take into account the interphase exchange of mass, momentum and energy, including the Stokes and Saffman forces, heat transfer, droplet evaporation etc. For disperse-phase concentrations considered in the present paper, the reverse effects of droplets on the carrier-phase motion are not significant and can be neglected, so that a one-way procedure of interphase coupling is actually used. More details of the mathematical model used and the numerical approach to simulation of motion of liquid droplets in a supersonic gas flow can be found in.

III. Nozzle and plume flow computations

A. Problem formulation

In this Section, the flow inside and outside an axisymmetric converging/diverging nozzle is considered. A schematic of nozzle geometry is shown in Fig. 2.

![Figure 2. Geometry of a supersonic conical nozzle.](image)

Flow computations are performed for two different conical nozzles, which will be hereafter referred to as Nozzle 1 and Nozzle 2. Nozzle 1 is the nozzle used by Rothe\textsuperscript{11} in his experiments on the low-Reynolds-number nozzle flows, while Nozzle 2 is from the recent experiments of Yarygin et al.\textsuperscript{5,12} performed at the Institute of Thermophysics (Novosibirsk). The geometric parameters of the nozzle and flow conditions for both cases considered are listed in Table 1.

Here the Reynolds number is defined as \( \text{Re} = \rho_0 u_m R_e / \mu_0 \), where \( R_e \) is the nozzle-throat radius, \( u_m \) is the maximum adiabatic velocity, and \( \rho_0 \) and \( \mu_0 \) are the density and viscosity in the plenum chamber, i.e.,
Table 1. Geometric Parameters and Flow Conditions of Conical Nozzles

<table>
<thead>
<tr>
<th></th>
<th>Nozzle 1 (Rothe’s experiments)</th>
<th>Nozzle 2 (Inst. of Thermophysics)</th>
</tr>
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<tbody>
<tr>
<td>Throat radius, ( R_t )</td>
<td>2.55 mm</td>
<td>5 mm</td>
</tr>
<tr>
<td>Exit radius, ( R_e )</td>
<td>20.92 mm</td>
<td>9.55 mm</td>
</tr>
<tr>
<td>Half angle of the</td>
<td></td>
<td></td>
</tr>
<tr>
<td>diverging part, ( \alpha )</td>
<td>20°</td>
<td>7°</td>
</tr>
<tr>
<td>Carrier gas</td>
<td>( N_2 )</td>
<td>( N_2 )</td>
</tr>
<tr>
<td>Stagnation temperature, ( T_0 )</td>
<td>300 K</td>
<td>293 K</td>
</tr>
<tr>
<td>Stagnation pressure, ( p_0 )</td>
<td>945 Pa</td>
<td>3990 Pa</td>
</tr>
<tr>
<td>Reynolds number, ( Re )</td>
<td>590</td>
<td>10,460</td>
</tr>
</tbody>
</table>

under stagnation conditions. The flow in Nozzle 2 is significantly denser than that in Nozzle 1, with much thinner boundary layer and a large inviscid core.

B. Numerical simulation of the gas flow inside the nozzle

The Navier-Stokes solver and hybrid NS/DSMC approach have been applied to calculate the flow inside the nozzle. The Navier-Stokes flowfields obtained for both Nozzle 1 and Nozzle 2 are shown in Fig. 3.

![Figure 3. Mach number flowfield for Nozzle 1 (left) and Nozzle 2 (right).](image)

It can be seen that for Nozzle 1 a thick boundary layer develops on the nozzle wall, so that the nozzle flow is fully viscous, with an only small inviscid core. For Nozzle 2, the boundary layer is much thinner and the inviscid core occupies the most part of the nozzle. Another typical feature of the latter flow is the compression fan emanating from the junction of the diverging part and the nozzle-throat rounding. When approaching the axis, this fan gradually transforms into a weak shock wave that reflects from the axis and then falls again on the nozzle-wall boundary layer.

The results of nozzle-flow computations performed with the Navier-Stokes solver and with the hybrid approach compare favorably both with each other and with experimental data. A detailed comparison has been performed for Nozzle 1. Figure 4 shows the density and temperature distributions along the centerline (axis) and Fig. 5 shows the density and temperature profiles near the nozzle-exit section.

It is evident that all solutions presented converge closely with the experimentally measured distribution along the nozzle centerline. As concerns the profiles in the vicinity of the nozzle exit, there are some noticeable differences. In particular, for this low-Reynolds-number flow, the temperature obtained from the solution of the Navier-Stokes equations with the no-slip boundary conditions differs from the experimental results almost everywhere and yields a much higher value of temperature near the wall. The use of slip boundary conditions, Eq. (1), significantly improves the agreement with experimental measurements.

C. Expansion flow around the nozzle lip

Of particular interest for the objectives of the present paper is the backflow in which some fluid particles leaving the nozzle turn by more than 90° and move in the opposite direction to the main part of the plume. The flow around the nozzle lip is critically important for backflow formation. To study this phenomenon,
hybrid NS/DSMC simulations of gas exhaustion from Nozzle 1 with three types of lips were performed: with an absolutely sharp lip, with a lip rounded with a radius of $1.67 \cdot 10^{-4}$ m, which is $0.134R_*$, and with a lip of radius $6.11 \cdot 10^{-4}$ m or $0.489R_*$.

The initial data for computations were taken from the previous Navier–Stokes simulations of the flow in the nozzle and in the plume exhausting from the nozzle. The plume entering the computational domain through the surface of a certain shape was identified within the field of parameters obtained previously. The flow computation near the nozzle lip was continued starting from this surface.

Figure 6 shows the density flowfields (normalized to the density under the stagnation conditions) for the gas leaving the nozzle for three radii of lip rounding. When the flow leaves the nozzle lip, the density drastically decreases (by several orders). The most interesting and somewhat paradoxical fact is that the density flowfields for all three shapes of the nozzle lip are almost identical.

More information about backflow formation can be extracted from the streamlines plotted in Fig. 7. The flow really turns at the nozzle lip at a large angle, and a backflow is formed. The backward streamlines seem to be diverging from one point at the nozzle lip. Careful consideration of streamlines inside the nozzle shows that the entire gas entering the backflow comes from a very thin near-wall layer. In our computations, this layer was located within one computational cell closest to the wall. Thus, the gas flow rate in the backflow should be quite small.

It is of interest to note again that the lip shape has almost no effect on the flow: the streamlines are almost identical for the three nozzles under study.

The backflow mass rates normalized to the total flow rate through the nozzle are $F_{\text{back}}/F_{\text{tot}} = 1.4 \cdot 10^{-3}$, $1.2 \cdot 10^{-3}$, and $9.5 \cdot 10^{-4}$ for the sharp nozzle lip, for the rounding radius of $1.67 \cdot 10^{-4}$ m, and for the
Thus, based on the results of simulations of gas exhaustion into vacuum from conical nozzles with three different radii of rounding of the exit lip, we can arrive at an important conclusion. In contrast to what could be expected, the change in the rounding radius of the nozzle lip retains the flowfield outside the nozzle almost unchanged. As for the backflow, the flow rate of the gas arriving at the back side of the nozzle is approximately $10^{-3}$ of the total flow rate through the nozzle.

Additionally, the flow simulation is performed with a screen located at a certain distance over the nozzle lip — see Fig. 8. Such a screen does not interfere with the flow originating from the nozzle boundary layer, but it eliminates the backflow from the plume. It results in a substantial change in the total backflow. Figure 9 shows the flow density as a function of the distance from the nozzle lip taken along the vertical line just left to the screen. The presence of the screen leads to a very significant decrease in density on the left side of the screen. It means that the most part of the backflow gas comes from the plume rather than from the nozzle boundary layer. It can be assumed that the mechanism of backflow origination from the plume is purely kinetic — molecules on the plume periphery gain an oppositely directed velocity owing to intermolecular collisions.

Hybrid NS/DSMC computations of the flow around the nozzle lip were also performed for Nozzle 2. The nozzle lip was rounded with the radius $1.67 \cdot 10^{-4}$ m. The density flowfield and streamlines for this case are shown in Fig. 10. In general, the flow structure is not changed significantly, though a twofold increase in the backflow mass flux should be noted: $F_{\text{back}}/F_{\text{tot}} = 2.5 \cdot 10^{-3}$ at the present conditions.
D. Droplet motion in the nozzle/plume flow

The flowfields obtained as a result of continuum and hybrid simulations are used to calculate the droplet motion inside the nozzle and in the plume. The computations are performed for Nozzle 2. Droplets of different sizes are introduced into the flow in the nozzle throat or in some cross section not far from the nozzle exit and traced with the Lagrangian algorithm described above. Figure 11 shows the Mach number flowfield, flow streamlines, and droplet trajectories for droplets of two different radii: \( r_p = 1 \) and \( 10 \) \( \mu \text{m} \). In contrast to the gas flow, droplets do not turn by a large angle near the nozzle lip, and there are no signs of the droplet backflow. Obviously, aerodynamic forces from the rarefied backflow are not sufficient to turn droplets sharply around the nozzle lip. The initial position of droplets (at the nozzle throat or closer to the nozzle exit) does not exert any substantial effect on their further motion. Even a small droplet placed initially within the wall boundary layer close to the exit section acquires large streamwise components of momentum, and the direction of its momentum vector cannot be immediately changed by the gas exposed to rapid expansion around the nozzle lip.

In order to obtain droplet phase distributions in the plume flow, a series of computations has been performed with varied droplet sizes. The droplets were initially uniformly distributed across the nozzle-throat cross section and had zero relative velocities. The number of probe particles was 5000 for each droplet size. The angular distributions of the liquid particles were registered at the surface corresponding to the outflow boundary of the Navier-Stokes computational domain, which was located far enough from the nozzle exit. Figure 12 shows the mass flux of particles on the outflow boundary surface as a function of \( \theta \), the angle measured from the nozzle axis.

As is evident from the numerical distributions, the flux of large droplets is confined in the range of angles of a few degrees, whereas smaller particles are dispersed at angles up to 30°. The mass flux of the liquid
Figure 10. Density flowfield (left) and streamlines (right) in the nozzle lip region for Nozzle 2.

Figure 11. Mach number flowfield, flow streamlines, trajectories of droplets coming from the nozzle for $r_p = 1 \mu m$ (left) and $10 \mu m$.

phase has a maximum at the plume axis and tends to a minimum at angles of approximately $30^\circ$ from the plume axis. It reproduces the experimentally observed behavior of angular distributions. However, the droplet distributions measured in the experiments have a second maximum corresponding to angles of $\approx 60^\circ$ off the centerline and also have a backflow component of the liquid phase up to angles of $\approx 135^\circ$. This range of droplet dispersion is not predicted by numerical simulations with the droplets originating inside the nozzle.

Thus, following the results obtained, it can be assumed that all droplets dispersed by large angles, in particular, droplets in the backflow, are coming not from the nozzle interior. A possible origin of such droplets may be disintegration of the near-wall liquid film at the nozzle lip, where the pressure rapidly decreases and the liquid becomes overheated. In fact, it was already supposed in. The process of disintegration is complicated and is caused by interaction of inertial, viscous, surface, gas-dynamic, and other forces. It is obvious that a competition of these forces is caused by the influence of the basic physical properties of the liquid (saturated vapor pressure, evaporation heat, surface tension, and viscosity), the parameters of the co-current gas flow (relative velocity, nozzle shape, pressure, and temperature), and the shape of the nozzle lip. Despite the complexity of physical processes involved in gas/droplet flow expansion into vacuum and liquid film disintegration, it is critically important to perform a numerical assessment of the dynamics of droplets originating near the nozzle lip. For this purpose, we conducted a set of numerical computations with droplets emerging near and outside the nozzle lip.

The droplets were initially uniformly distributed on the torus surface “wrapping” round the nozzle lip; the distance from the nozzle lip to the torus surface was $r = 0.5$ mm. The nozzle lip here was rounded with radius $r = 0.167$ mm. The computed droplet traces are shown in Fig. 13. It is quite clear that the droplets acquire a large enough cross-streamwise velocity component to “fly away” into the far field of the plume.

It is obvious that the droplets in this case penetrate deeply into the backflow region. The trajectories of the lightest droplets considered make angles up to $140^\circ$ to the nozzle plume direction. This value agrees surprisingly well with the available experimental data.
There is still too much ambiguity in the initial distribution of the droplets (their initial locations, velocities, etc.) in this case to make a direct quantitative comparison of the computation results with the experimental data on the distribution of droplet-phase mass. Moreover, the relative disperse-phase mass fluxes of the droplets emerging inside the nozzle and the droplets formed near the nozzle exit are not known a priori. Nevertheless, we believe that the correlation obtained between the results of computations and the experimental data is really encouraging.

We can now conclude that the spatial distribution of the disperse phase observed in the experiments consists of two basic parts: the flux of droplets emerging inside the nozzle (most likely, due to rapid flow acceleration and sharp deflection of the near-wall film in the nozzle throat) and the droplets originating near the nozzle lip (due to rapid expansion of the flow into vacuum). Indeed, these two flow regions have the largest gradients of flow parameters. These are, therefore, the most probable locations where the liquid film breakup could occur.

IV. Simulations of the flow over an expansion corner

Based on the results described above, it is evident that the investigation of flow expansion around the nozzle lip is critically important for studying backflow contamination. For an inviscid flow, it is well known from the Prandtl-Meyer solution that there is a limiting flow deflection angle. At this limiting angle, all internal energy of the gas transforms to kinetic energy of motion, so that the flow temperature becomes zero while the Mach number grows up to infinity. The viscosity effects can change the expansion flow substantially.
and, in particular, they favor flow turning by large angles and backflow formation. To investigate this phenomenon in more detail, we consider here a model problem consisting of the flow over an expansion corner formed by a plane wall (flat plate) suddenly deflecting by a large angle. As a limiting case, where the wall deflection angle reaches 180°, flow turning around the trailing edge of the infinitely thin flat plate is obtained. For the first time, a similar model problem was considered by Bird\(^8\) who established a number of important features of such a flow. In particular, he demonstrated that the sonic line, which separated the subsonic part of the flat-plate boundary layer from the supersonic one, terminated at the corner vertex (nozzle lip), so that the subsonic part of the boundary layer was closed.

The flow geometry is shown in Fig. 14. The wall deflection angle \(\varphi_w\) is varied in different simulations. To exclude any influence of models governing the exchange between translational and internal degrees of freedom of molecules, a monatomic gas (\(\gamma = 5/3\), Argon) is considered in this Section. Further, the problem under consideration is simulated with two types of wall boundary conditions: inviscid conditions (non-permeability for Navier-Stokes simulations, specular reflection for DSMC) and viscous conditions (slip conditions, Eq. (1), for NS, diffuse reflection for DSMC). It allows us to distinguish between the viscosity effects in the expansion flow itself and those related the viscous boundary conditions and flow deceleration within boundary layers.

![Figure 14. Schematic of the flow over an expansion corner.](image)

The simulations are performed for the following flow parameters: the inflow Mach number \(M_\infty = 4.38\) and static flow temperature \(T_\infty=75\) K. The Reynolds number based on the distance \(L\) from the leading edge of the boundary layer to the expansion corner is varied \(Re = 476, 4760, 47600\) to investigate the effects of flow viscosity. The flow was simulated by the DSMC method and with the Navier–Stokes equations. The Navier–Stokes computations were performed for the expansion corner of \(\varphi_w = 37.1^\circ\), which coincides with the maximum Prandtl–Meyer angle \(\varphi_{\text{max}}\) for \(\gamma = 5/3\) and \(M_\infty = 4.38\). Note, the maximum Prandtl–Meyer angle for \(\gamma = 5/3\) and \(M_\infty = 1\) is 90°. The DSMC computations were performed with \(\varphi_w = 37.1^\circ\) and also with \(\varphi_w = 180^\circ\), the latter simulates expansion into vacuum around the nozzle lip. The flow was assumed to be two-dimensional.

### A. Simulation with inviscid boundary conditions

In the first series of computations the inviscid boundary conditions (non-permeability for Navier-Stokes simulations, specular reflection for DSMC) were used on both walls (Wall 1 and Wall 2) to elucidate the net effect of viscosity on expansion flow without the influence of boundary layers. The typical flowfields obtained are shown in Fig. 15. These computations were performed at the Reynolds number \(Re = 47600\), the wall deflection angle in the DSMC simulation was \(\varphi_w = 180^\circ\).

A close resemblance of two flowfields is worth noting, it holds in spite of the different shape of the computational domains used. Further, it is evident from the flowfields that the numerical solutions are close to the classical Prandtl–Meyer solution only in some range of polar angles \(\varphi\) (here \(\varphi = 0\) corresponds to the axis going along Wall 1, and \(\varphi\) is positive in the clockwise direction). Another interesting feature of the solutions obtained is a non-monotonous behavior of the Mach number: starting from some \(\varphi\) it begins to increase.

The angular distributions of the flow parameters (non-dimensional density \(\rho/\rho_\infty\), Mach number, temper-
Figure 15. Navier–Stokes (top) and DSMC (bottom) Mach number flowfields for the flow over an expansion corner.

ature $T/T_\infty$ and the flow velocity normalized on maximum adiabatic velocity $|\vec{u}|/u_m$ are given in Fig. 16. These distributions were recorded along the circle with radius $r/L = 0.4$ centered at the vertex of the expansion corner. For comparison, the inviscid Prandtl–Meyer analytical solution is also plotted in the figures. The DSMC computations in this case were performed for wall deflection $\varphi_w = \varphi_{\text{max}} = 37.1^\circ$ and also for flow expansion into vacuum around the trailing edge, i.e. for wall deflection $\varphi_w = 180^\circ$.

It is evident that the flow viscosity substantially changes the flow around the corner even if the inviscid wall boundary conditions are imposed. This is manifested in termination of growth of the flow Mach number at some polar angle, whose value depends on the Reynolds number, and also in an excessive increase in flow temperature compared to the Prandtl–Meyer solution. These changes become more apparent as the flow Reynolds number decreases. Note, the flow parameters tend to their inviscid limit with increasing Reynolds number.

The results of DSMC computations with different wall deflection angles ($\varphi_w = 37.1^\circ$ and $180^\circ$) are very close to each other. This is probably explained by the fact that the flow density is almost zero for $\varphi = 37.1^\circ$. Beyond this value, the flow is basically free-molecular. It should be noted that $\varphi_{\text{max}}$ is based on the inviscid theory and does not necessarily hold in this case where the viscous forces produce their effects. Still, in the absence of the boundary layers on the walls that form the expansion corner, the inviscid theory predicts the maximum turning angle quite well. Nevertheless, the density in the Navier–Stokes computations performed with $\text{Re} = 476$ is quite different from zero even for $\varphi = \varphi_{\text{max}}$. This case, $\text{Re} = 476$, demonstrates the most prominent differences of the Navier–Stokes results compared to the DSMC computations. These differences are evident in this case from the very beginning of flow expansion. The flow Mach number in Navier–Stokes computations does not grow at all. This is caused by the growth of flow temperature due to the work of viscous forces. Based on this, we can conclude that the Navier–Stokes equations are not applicable to simulation of flow expansion at such a low Reynolds number For higher Reynolds numbers, i.e., for $\text{Re} = 4760$ and $\text{Re} = 47600$, the Navier–Stokes results are in close agreement with the DSMC computations up to the polar angles $\varphi \approx 5^\circ$ and $\varphi \approx 15^\circ$, respectively.
Figure 16. Angular distribution of density, Mach number, temperature, and velocity around the expansion corner with inviscid wall boundary conditions.

B. Simulation with viscous boundary conditions

To investigate the influence of wall boundary layers, the computations were also performed with the viscous boundary conditions on Wall 1: velocity slip and temperature jump conditions in Navier–Stokes computations, and diffuse reflection with the energy accommodation coefficient \( \alpha_c = 1 \) in DSMC computations. The wall temperature was \( T_{w1} = 300 \text{K} \), and the Reynolds number was \( \text{Re} = 4760 \). The turning angle in the Navier–Stokes computations was \( \varphi_w = 90^\circ \) in this case. On Wall 2 where the flow is very rarefied, the inviscid boundary conditions are imposed again. Since the flow in the boundary layer upstream of the expansion corner has a much lower Mach number than \( M_\infty = 4.38 \), we can expect that the maximum turning angle in this case would be close to \( \varphi_{\text{max}} = 90^\circ \) predicted for \( M_\infty = 1 \) flow of an inviscid monatomic gas. The DSMC computations were conducted for \( \varphi_w = 180^\circ \) turn. The corresponding polar distributions of flow parameters along the circle of radius \( r/L = 0.5 \) are plotted in Fig. 17.

It is evident that the boundary layer on the wall upstream the expansion corner indeed favors flow deflection at a higher angle. The density becomes close to zero at \( \varphi \) in the range 60-70 degrees. The temperature and, consequently, the Mach number obtained in the Navier–Stokes computations become apparently different from the DSMC results, starting from \( \varphi \approx 0 \). What is most important is that the non-physical temperature growth in the Navier–Stokes computations is almost unlimited (the zero gradient of temperature at \( \varphi = 90^\circ \) evident in Fig. 17 is actually the influence of the zero-gradient boundary conditions imposed on the wall located at \( \varphi = 90^\circ \)). On the contrary, in DSMC computations, the flow temperature tends to its frozen value as the flow is expanded.

We can conclude that the use of the combined Navier–Stokes/DSMC approach for simulation of the gas-
Figure 17. Angular distribution of density, Mach number, temperature, and velocity around the expansion corner with viscous wall boundary conditions.

droplet flow around the nozzle lip is essentially important since the Navier–Stokes approach become no longer acceptable as the flow is expanded. Moreover, the excessive non-physical growth of flow temperature observed in the Navier–Stokes computations may cause qualitatively different results in the regions of low-density flow since the gas/droplet interaction (heat flux, evaporation) processes are dependent on the temperature of the ambient gas.

In general, the boundary layer on the plate favors backflow formation. The Mach number around the trailing edge reaches its maximum value near the streamline passing along the outer edge of the boundary layer. The results of Navier-Stokes and DSMC computations agree very well up to the polar angle $\varphi = 10^\circ$ in this case. At higher angles, the Navier-Stokes computations demonstrate a rapid increase in flow temperature, which is probably non-physical.

V. Conclusions

A detailed numerical investigation of the backflow formation phenomenon for nozzle plumes expanding into vacuum has been performed by a hybrid approach combining the continuum (Navier-Stokes) and kinetic (DSMC) computations. Two different conical nozzles used in earlier experimental studies have been considered. The flow around the nozzle lip has been investigated in detail for different shapes of the nozzle lip (sharp and rounded). It has been found that the mass flow rate in the backflow region is rather small, amounting approximately to $10^{-3}$ of the total mass flux through the nozzle. The simulation also demonstrate that intermolecular collisions in the plume peripheral zone contribute substantially to formation of the low-density backflow.
The motion of small droplets immersed in the flow has been investigated using a Lagrangian particle algorithm coupled with continuum carrier gas flow computations. It has been shown that aerodynamic forces are not sufficient to turn droplets from the nozzle interior around the nozzle lip and drag them in the backflow. At the same time, droplets emerging in the vicinity and outside of the nozzle lip follow the gas flow and penetrate deeply into the backflow region. It means that the source of reverse flow of droplets observed in some experiments can be disintegration of the cooling liquid film on the nozzle lip rather than droplet entrainment from the nozzle interior.

The viscous expansion flow over an expansion corner has been investigated to elucidate details of backflow formation near the nozzle lip. The results of Navier–Stokes and DSMC simulation have been compared and analyzed. It has been found that the effects of viscosity become more significant with the flow expansion and dominate in the rarefied regime. The influence of viscous dissipation causes a decrease in the Mach number and a growth of temperature in contrast with the inviscid Prandtl–Meyer solution.

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