Modeling of a Small Hydrazine Thruster Plume in the Transition Flow Regime

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Three different techniques commonly employed in the calculation of rocket and thruster expansion plumes are assessed. These techniques vary both in computational expense and in the accuracy and detail of the solutions that they provide. The assessment is made with reference to the plume expanding from a small monopropellant hydrazine thruster and includes comparison with experimental data. Two of the modeling techniques, the Simons model and the Method of Characteristics, rely on the continuum equations. The third, the Direct Simulation Monte Carlo method (DSMC), adopts a discrete particle approach. The validity in employing continuum methods in the flowfield between the continuum and free molecular limits (i.e., the transition flow regime) is investigated. It is noted that the more computationally intensive DSMC solution method is the proper technique in this region of the expansion plume. Additional results provided solely by the DSMC calculations, such as thermal nonequilibrium effects, are presented. The consequences arising from the apparent differences in the results obtained with the continuum and discrete particle methods at the free molecular limit are assessed in terms of impingement effects.

Introduction

SPACECRAFT are usually controlled by jets exhausting from thrusters into the near vacuum of space. Because of the very low external pressures encountered, these plumes expand into such large solid angles that backflow must be properly considered. The interaction between the plume constituents and spacecraft surfaces are therefore numerous and lead to such deleterious impingement effects as torques affecting the attitude of the spacecraft and contamination of sensitive surfaces.

These events will have the result of reducing the effective lifetime of the spacecraft so that detailed prediction of their occurence is of great importance in the design stages of any spacecraft.

Maintaining laboratory pressures low enough to simulate the space environment is very costly, and presents many technical difficulties. In the absence of reliable theoretical predictions, spacecraft engineers have tended to use highly conservative estimates of plume impingement effects. Further progress in this area would clearly lead to better optimization in the design process.

In the plumes exhausting from small thrusters, rarefaction effects are particularly important. In addition, relaxation and freezing of internal energy modes, condensation, and chemical reactions may all take place.

It should be noted that the expansion plume may be divided into three distinct flow regimes, which are essentially characterized by density. As a streamline is followed along its path from the nozzle exit into the ambient vacuum, there is a rapid reduction in the gas density. The high densities associated with the nozzle place flow at the exit in the continuum regime. As the streamline proceeds, a point is reached at which the continuum equations become invalid. The transition flow regime is then entered. Further travel along the streamline leads eventually to collisionless flow.

The decrease in the density associated with the transition flow regime leads to a reduction in the molecular collision rate of the gas. Eventually the collision rate reaches a level where thermal equilibrium can no longer be maintained and the continuum equations become invalid. The nonequilibrium nature of the transition flow regime is typically seen in the separation of the axial and radial components of the translational temperature.

The breakdown of the continuum equations may be characterized by Bird's parameter:

$$P=\frac{u}{\rho v}\left|\frac{d\rho}{ds}\right| \tag{1}$$

where u is the stream velocity, ρ is the density, v is the collision frequency, and s is the distance along a streamline. The onset of transition flow occurs when P has a value of approximately 0.05.[2] The same parameter may also be used to identify the point at which free molecular flow begins. Here, the parameter is usually taken to have a value of 2.

Before undertaking any calculations, the degree of detail required from the investigation should be determined and balanced against the computational cost involved in processing the results. In the present work, the modeling of combustion processes and the expanding nozzle flow is undertaken in a simplistic manner. The primary focus of the investigation is the expansion of the thruster plume.

The most popular methods used in exhaust plume prediction are the Simons model,[3] the Method of Characteristics (MOC)[4] and the Direct Simulation Monte Carlo method (DSMC).[5] The Simons model provides an analytic expression for the density as a function of the position in the flowfield and therefore incurs little computational expense. Results of good spatial resolution using MOC calculations necessitate a moderate amount of CPU time by comparison. Both these techniques rely on continuum equations, so that their use in the transition regime is incorrect.

Although it is certainly the most expensive of the three techniques considered, the DSMC method is the proper technique for calculating flow in the transition regime. In addition, the calculations provide information concerning thermal nonequilibrium and species separation effects. These properties cannot be investigated using continuum methods.

In previous work,[3,4] continuum calculations have been used throughout the transition regime and are used to identify the "freezing" surface, i.e., the point at which $P=2$. As stated already, this is incorrect. It is the aim of the present work to investigate the errors associated with such procedures by carrying out DSMC calculations throughout the transition regime. In particular, errors encountered with continuum calculations near the free molecular limit are analyzed and the subsequent effects on impingement calculations assessed. It is stressed that the calculation is made of freestream quantities

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only. Although such quantities are generally distorted in the presence of a spacecraft surface, they do provide a useful indicator of the likely impingement effects.

In this paper, results obtained in the isentropic core expansion are reported for each of the three modeling techniques. The expansion of the boundary layer has not been dealt with at this stage. The plume chosen to be modeled is that exhausting from a particular 0.5N hydrazine thruster.

Physical Considerations

The 0.5N hydrazine thruster is shown in Fig. 1; the dimensions are in millimeters. Since the nozzle wall is conical, there is no necessity to consider the possibility of compression shocks in this study. This particular thruster has been chosen for investigation for a number of reasons. Firstly, this thruster has been studied experimentally at DFVLR, Gottingen, Federal Republic of Germany.[6,7] It is, therefore, possible to validate the three sets of solutions obtained in this study against such data.

Another important feature of the thruster is its small size, which makes it more amenable to DSMC calculations. Although such a plume is certainly simpler than those produced by thrusters burning solid propellants[8] or bipropellants,[9] the decomposition of hydrazine into ammonia, nitrogen, and hydrogen does allow some investigation of species separation effects.

Whereas the Simons model and the MOC solution techniques have sufficiently low computational requirements to allow parametric investigations, the same cannot be said of the DSMC method. The solution corresponding to the available experimental data is therefore the only solution presented for each of the three modeling methods.

Details of the prevailing combustion chamber conditions, together with the plume gas properties, are given in Table 1 and have been obtained through the procedures described in Ref. 7. In all the calculations performed, it has been assumed that neither chemical reactions nor relaxation of vibrational energy modes occurs. This is in accordance with the theoretical study performed by Kewley[10] for the thruster under consideration. Kewley reports that the chemical and vibrational states of the gas were found to be effectively frozen at a point just beyond the nozzle throat.

Using the one-dimensional analysis of Gordon and McBride,[11] the nozzle exit temperature is estimated to be 160 K. It is evident that as the plume rapidly expands into the vacuum, very low temperatures will be encountered. In the case of both ammonia and nitrogen, the possibility of condensation is, therefore, very real. However, such considerations are beyond the scope of the current work. In addition, it is noted that the Pitot pressure probes employed in the acquisition of the experimental data are generally unaffected by condensation effects.

Continuum Calculations

Simons Model

An analytical model for the prediction of flow properties in rocket exhaust plumes was developed by Boynton[12] and Simons[13] several years ago. Specifically, this model introduces an expression for the density at a point in the axisymmetric flowfield described in polar coordinates, i.e.,

$$\rho(r,\theta) = \frac{A}{r^2} f(\theta) \tag{2}$$

where A is the plume constant. The following equation

$$f(\theta) = \cos^{\frac{2}{\gamma-1}}\left(\frac{2\theta}{\pi\theta_L}\right) \tag{3}$$

describes the angular density behavior, and θ_L is the limiting angle of the expansion.

The assumptions inherent in formulating Eq. (2) are as follows:

1) The streamlines are straight lines radiating from the point on the plume axis at the nozzle exit.

2) The velocity is everywhere constant and equal to the limiting value.

3) The density decreases radially.

The model divides the flowfield into two distinct regions in which the expansion of the boundary layer is treated separately from that of the isentropic core. In the latter, the one-dimensional isentropic relationships are employed together with the known stagnation conditions to derive all important flow quantities from Eq. (2). In the boundary layer, the concept of "effective" stagnation conditions is introduced. Under this process, the stagnation conditions are assumed to show an angular dependence. These ideas, together with details of procedures for the calculation of the plume constant from the gas type and nozzle geometry, are fully explained in Ref. 3.

The input data required by the Simons model are entirely described by the combustion chamber properties and the geometry of the nozzle. Because of the very low computational expense incurred by the model, it is ideally suited to parametric studies. In addition to the usual flow quantities, such as Mach number and temperature, it is also possible to derive values for the local mean free path, collision rate, and Bird's breakdown parameter, as given by Eq. (1).

The Simons model has achieved a certain degree of success and, due to its analytic nature, is a widely applied engineering tool. Calia and Brook[14] found good agreement for density measurements made at large angles from the plume centerline. Lengrand et al.[15] have investigated exhaust plumes of nitrogen for a number of small thruster nozzles. In this study, excellent agreement was found between theoretical prediction and experimental data for nozzle exit Mach numbers up to $Ma_E = 5$. These comparisons were made with reference to axial density and temperature ratios.

Calculations with the Simons model for nozzles having exit Mach numbers in excess of 5 have, however, been unsatisfactory. It is noted that the thruster under consideration has an exit Mach number of 5.78. In a recent publication, the model has been modified to emulate the nonradial expansion of such plumes.[16] The results of that study are not considered in the present work.

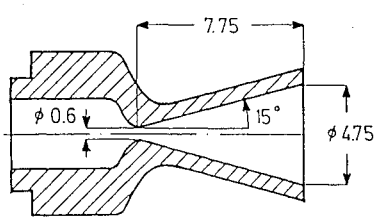


Fig. 1 The 0.5N hydrazine thruster.

Method of Characteristics

This well-known computational technique has been previously employed to model large rocket and thruster plume expansions.[3,8] However, the application of the method to small nozzles presents some difficulties. The MOC algorithm is derived from the Euler equations and should not be applied to viscous flow. As has already been explained, the 0.5N thruster considered here has a large laminar boundary layer associated with it. In the present work, the boundary layer is treated by assuming a velocity profile appropriate to laminar flow past a flat plate. The results of this procedure are not reported here, as they were found to have no bearing on the isentropic core expansion presently considered.

Another problem with the MOC technique lies in the acquisition of initial input data. The computations are usually begun at either the nozzle throat or the nozzle exit. As the noz-

Table 1 Prevailing combustion chamber conditions

Stagnation conditions		Exit plane properties	
Pressure, Pa	1.57×10^{6}	Mach number	5.78
Temperature, K	1170	Specific heat ratio	1.37
Viscosity, Nsm^{-2}	4.03×10^{-5}	Molecular weight	12.90

Gas properties

Molecular species	Mole fraction	Molecular weight	Reference collision diameter	Rotational degrees of freedom
H_2	0.4933	2	2.98×10^{-10}, m	2.00
N_2	0.2987	28	4.07×10^{-10}, m	2.00
NH_3	0.2080	17	4.86×10^{-10}, m	3.25

zle under consideration contains no compression shocks in the nozzle flow, the calculations are commenced at the nozzle exit. The program of Gordon and McBride[11] was used to calculate the exit plane data for the expansion of the decomposed hydrazine. A uniform distribution for the isentropic core at the nozzle exit was then assumed.

Results

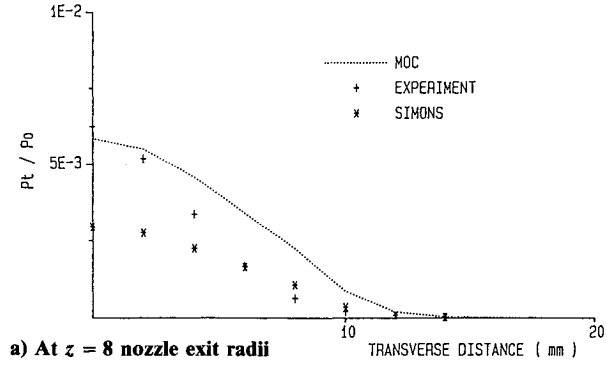
Transverse calculations of Pitot pressure have been made at several axial stations and are presented in Figs. 2a-2d. Included in these figures are experimental results obtained at DFVLR.[7] The results obtained near the nozzle exit are observed in Fig. 2a to be unsatisfactory for both calculation procedures. These profiles are obtained in that part of the flowfield where the limiting velocity has not yet been reached. This area is designated the nearfield of the expansion and extends to a distance no greater than 20 exit radii along the plume axis.[7] In the remaining three sets of profiles, it is clear that the MOC solutions offer greater correspondence to the experimental data. Table 2 lists the differences observed between the calculated and experimental data found at the plume axis as a function of axial distance. Two important features become apparent from this analysis. First, it is clear that the MOC and Simons model solutions are found to converge as we proceed along the axis. At the same time, it is found that the agreement between the experimental data and the MOC calculations diverge as we move downstream.

The barrel shock observed in the experimental data is a consequence of the presence of a finite background pressure in the laboratory.

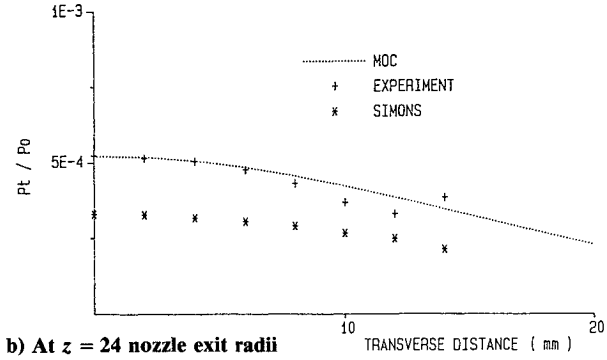
The primary objective in obtaining the solutions to expansion plumes is to enable prediction of possible impingement effects. In particular, the calculation of the forces resulting from the interaction of the plume with a spacecraft surface is of interest. The flow quantities relevant to such analysis are density, velocity, and, to a lesser extent, temperature. The results presented in the isentropic core of the plume expansion of the 0.5N thruster show that the important properties are predicted by the MOC calculations to be within about 13%. The results obtained with the Simons model do not correspond as well to the experimental data. However, the fact that the Simons model is more readily and efficiently applied to the calculation of the effects of impingement with complex spacecraft structures suggests that it is a useful design tool.

Calculation of the two contours identifying the beginning and end of the transition flow regime has also been undertaken. As the Simons model is found to be less accurate, the contours were found using MOC calculations, and are displayed in Fig. 3. The point at which the continuum breakdown contour intersects the plume axis is found to lie at a distance of 22 exit radii downstream of the nozzle and is thus beyond the nearfield. Also, the MOC calculations that best correspond to the experimental data (Fig. 2b) are observed to lie close to the continuum regime. We may, therefore, be confident that the continuum limit has been accurately identified.

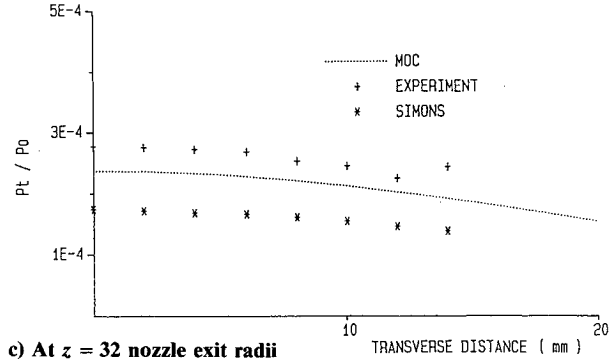
Figure 3 also demonstrates that the experimental investigation of Ref. 7, which reaches a maximum point downsteam of



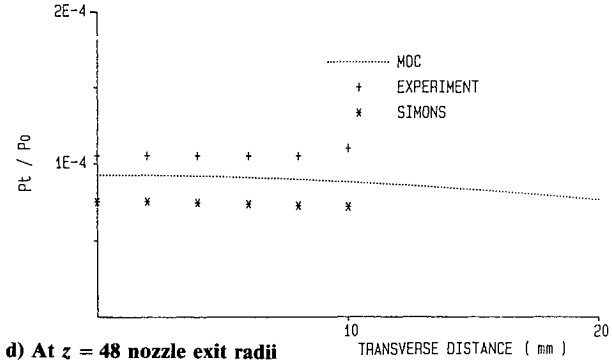
a) At z = 8 nozzle exit radii



b) At z = 24 nozzle exit radii



c) At z = 32 nozzle exit radii



d) At z = 48 nozzle exit radii

Fig. 2 Transverse Pitot pressure distributions.

Table 2 Difference between calculated and experimental data

Axial station (exit radii)	Ratio of results (MOC/experiment)	Ratio of results (Simons/experiment)
8	0.9142	0.6223
24	0.9925	0.7490
32	0.8973	0.7538
48	0.8712	0.7664

48 exit radii, covers a small fraction of the total transition flow regime. The trends observed in Figs. 2 and Table 2 for the correspondence between calculated and experimental data indicate that significant errors may be associated with the determination of the location of the free-molecular limit. This aspect of the calculations is investigated using the discrete particle approach.

Direct Simulation

Method

The DSMC method developed by Bird[5] is a computational technique in which the large number of molecules in a real gas is simulated by a much smaller population of representative particles. The number of these particles is typically in the thousands, and their trajectories and intermolecular collisions are simultaneously calculated in the region of physical space to be modeled. The computational expense of the method is found to be inversely proportional to the density of the flow. Thus, application of the technique has been almost entirely limited to those in the near-continuum and transitional flow regimes. A network of cells encompassing the flow domain must be calculated prior to simulation and is used to ensure that the smearing of local flow gradients is prevented and is also used for the sampling of flowfield data. All collisions are calculated on a probabilistic basis so that any solution is essentially unsteady. However, a steady solution is found by the large time state of these unsteady results. Whereas velocity space is always treated in three dimensions, flow symmetries are often used to reduce the number of grid dimensions. Many important physical phenomena may be modeled using the DSMC technique including relaxation of internal energy modes, chemical reactions, and gas-surface interactions.

In the calculation of the hydrazine thruster plume, the flow is taken to be axisymmetric. As the chemical and vibrational states of the flow are assumed to be frozen, these phenomena are not included. Exchange of energy between translational and rotational energy modes is simulated through the use of the Borgnakke-Larsen phenomenological model.[17]

The flow domain to be simulated is described by the flow limits shown graphically in Fig. 3. Having identified the transition regime, the construction of a suitable computational grid must be considered. This has been accomplished by using the continuum MOC calculations to make local estimates of mean free path. The grid spans the isentropic core of the expansion plume, as predicted by the Simons model. This region

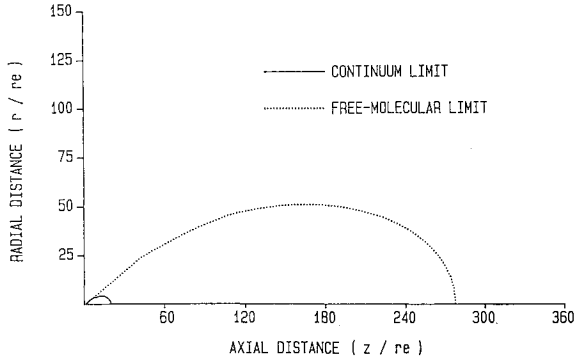


Fig. 3 Breakdown contours defining the transition flow regime.

of the flowfield was also found to be unaffected by variations in the laminar velocity profile assumed for the MOC calculations. Molecules are released into the simulation region across both the continuum breakdown locus and the upper boundary of the grid. The initial flow properties are sampled from the equilibrium distribution functions appropriate to the local flow conditions provided by the continuum solutions.

The large differences in mean free path and collision rate in the extremities of the flowfield are treated through the use of different discrete time-steps and physical scaling factors.

The DSMC method employed to simulate the collisional processes has been the subject of some recent debate. In the solution of rarefied gas flows, the Boltzmann equation is generally regarded as the most appropriate mathematical model. The most commonly employed DSMC scheme is the Time Counter method of Bird.[5] Whereas the Boltzmann equation may be derived from Bird's collision scheme, the reverse is not true. Since Nanbu[18] has derived a scheme directly from the Boltzmann formula, it would be expected that his method would be preferred. However, in a comparison of these DSMC schemes, the authors have shown [19] that, in addition to much greater numerical efficiency, Bird's method is also more flexible in terms of the choice of initial simulation parameters. In any case, as stated by Bird,[20] it is the physics of the flow rather than the peculiarities of a particular mathematical model that should determine the appropriate simulation scheme.

Results and Discussion

In Figs. 4-6 are shown some typical DSMC results together with calculations made with the MOC. Figure 4 compares total temperature contours. Whereas the results agree near the continuum limit, they are observed to diverge through the transition regime. Near the "freezing" surface the two methods are seen to give a discrepancy of about 100%. Figure 5 shows axial and radial temperature contours that may only be obtained from the DSMC solution. The divergence of these contours indicates the degree of thermal nonequilibrium in the flowfield. In Fig. 6 are shown results for rotational and translational temperature. Once again it is clear that these thermal modes are not in equilibrium.

In Fig. 7, Pitot pressure calculations are plotted as a function of position at a radial distance of 48 exit radii from the nozzle exit. Included are experimental data and continuum predictions. It is clear that the DSMC results more closely resemble those obtained in the laboratory. Figure 8 shows the solutions for total temperature along the same locus. The predictions provided by the two methods are seen to differ slightly, with those calculated using direct simulation being lower than the corresponding continuum values.

For the small dimensions of the considered thruster, most impingement studies will involve the use of flow properties derived at the free molecular limit. This is located at about 68 cm from the nozzle exit. In Fig. 9, the ratio of MOC to DSMC solutions for several flow quantities are plotted along the locus defining the onset of collisionless flow. It is clear that disparities exist for each of the properties derived at the free molecular limit. This is located at about 68 cm from the nozzle exit. In Fig. 9, the ratio of MOC to DSMC solutions for several flow quantities are plotted along the locus defining the onset of collisionless flow. It is clear that disparities exist for each of the properties considered.

In terms of the mean free path calculated by the two methods, the direct simulation results tend to be smaller than those predicted from MOC. In accordance with this finding, the DSMC calculations are extended beyond the $P=2$ locus, which was determined from the MOC results.

The divergence in the results obtained from total temperature by the continuum and discrete methods is also apparent in Fig. 9. The extremely low temperatures predicted in this part of the flowfield give rise to very large molecular speed ratios, typically in excess of 40. As a consequence, the large differ-

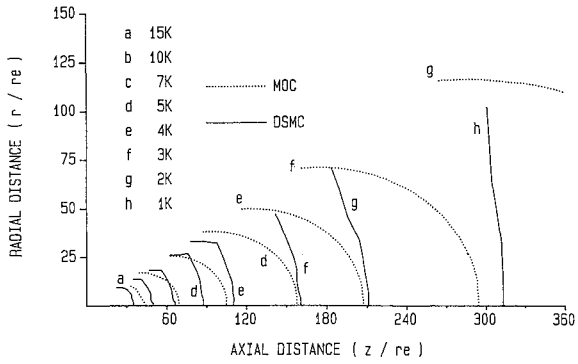


Fig. 4 Comparison of MOC and DSMC solutions for total temperature.

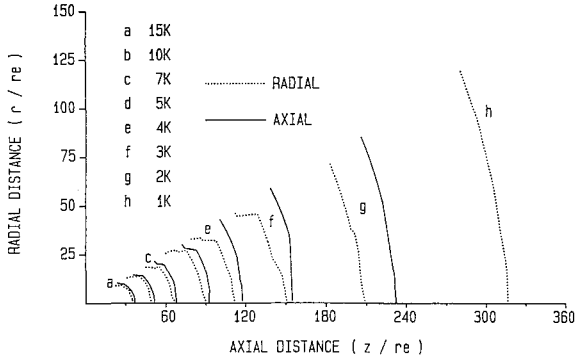


Fig. 5 DSMC solutions for axial and radial temperature.

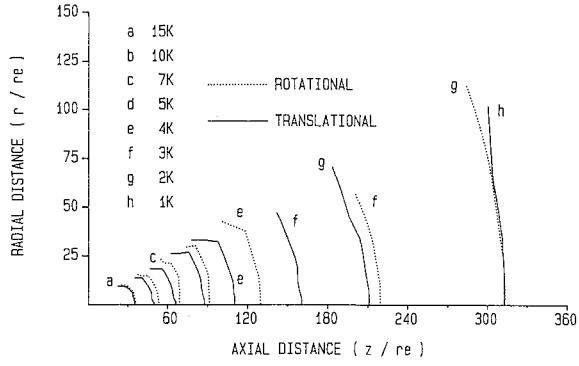


Fig. 6 DSMC solutions for translational and rotational temperature.

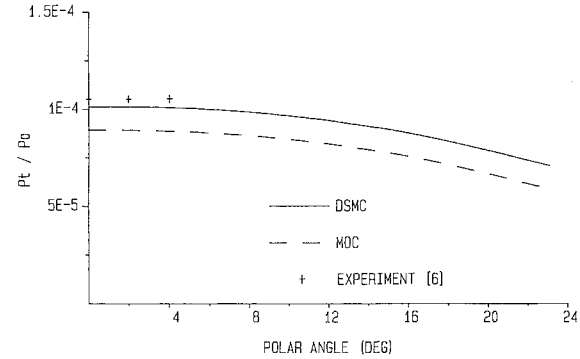


Fig. 7 Pitot pressure solutions along the radius $r = 48$ nozzle exit radii.

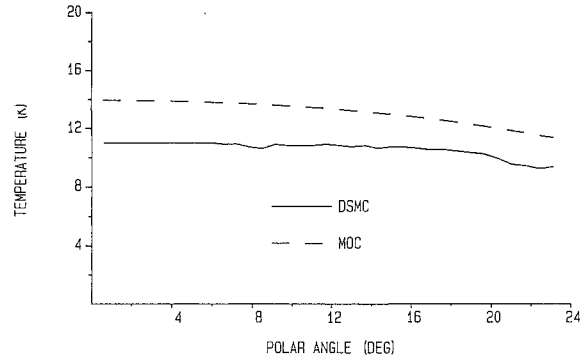


Fig. 8 Total temperature solutions along $r = 48$ nozzle exit radii.

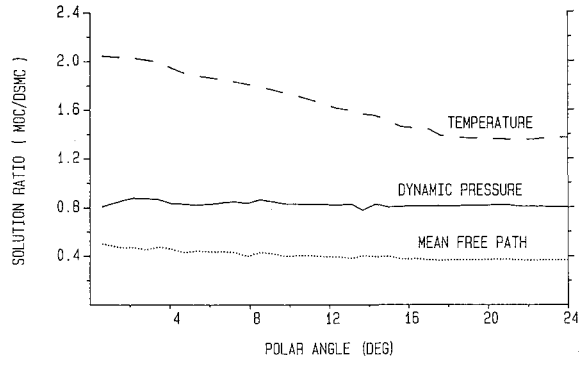


Fig. 9 Solution ratios (MOC:DSMC) along the free-molecular locus.

ences in temperature prediced by the two methods, as much as a factor of 2, translate into very small deviations in aerodynamic force coefficients. In the case of drag coefficient on a flat plate, this amounts to less than 1%.

The local flow angle is another quantity that directly affects the calculation of impingement effects. The small disagreement found for the two sets of solutions was again found to have a negligible effect on both drag and lift coefficients.

The quantity most relevant to impingement analysis is the dynamic pressure given by $1/2\ \rho u^2$. For the small thruster under consideration, the limiting velocity of the flow is reached within 20 exit radii of the nozzle exit. However, significant differences in density calculations were noted and are directly transferred to the solutions for dynamic pressure. These errors are found to be of the order of 20% and represent the total difference in impingement calculations based on MOC and DSMC freestream solutions at the free-molecular limit of the expansion. With the increasing demand for improved assessment of thruster fuel budgets, such errors are clearly important and highlight the usefulness of proper treatment of the transition flow regime.

Species separation effects may also be investigated with the DSMC technique. In the present application, these were found to be minimal due to the fact that the stream velocity is very much larger than the thermal velocities associated with the molecular species present in the flowfield.

For completeness, the solutions of the Simons model and direct simulation have also been compared at the free-molecular limit. These results are found to be similar to those shown in Fig. 9. The disagreement in dynamic pressure is calculated at about 28%. The values for temperature and mean free path are very close to those obtained in the MOC calculations. These results are to be expected from the trends observed in Table 2. They show that at the point where the flow becomes collisionless, little additional error is incurred by adopting the more economical Simons model instead of the MOC.

Conclusions

In the present work, results have been obtained for the expansion of the isentropic core of the plume exhausting into hard vacuum from a small hydrazine thruster. The calculations have been completed using three solution techniques which vary both in the accuracy and detail of the solutions provided. The two continuum methods assessed, the Simons model and the MOC, are commonly applied to the flow

regime lying between the continuum and free-molecular limits. This procedure is incorrect from a theoretical standpoint, as the Boltzmann equation, rather than the continuum equations, is the proper mathematical model in the transition regime. The DSMC method has therefore been used to provide the exact solution to the problem.

The solutions for Pitot pressure obtained with the Simons model and MOC calculations were compared with experimental data. The MOC results were found to offer significant improvements on those obtained with the simple analytical model. The Simons model predictions are found to be in error by up to a factor of 1.6. Although the MOC results offer excellent agreement with the experimental values, the correspondence between the two seems to diverge slightly as we proceed through the transition regime. It is also noted that the two sets of continuum solutions are found to progressively converge downstream of the nozzle.

The DSMC solutions for Pitot pressure agree with the experimental data, and offer slight improvements on the MOC calculations. At the free-molecular limit, the difference between the discrete particle and MOC results for impingement quantities is found to be about 20%. This error has important implications in the assessment of onboard fuel budgets and arises as a direct consequence of applying continuum equations in the transition flow regime.

Large differences in total temperature are noted for the DSMC and MOC calculations. At the onset of free-molecular flow, they are separated by a factor of 2. However, due to the very high speed ratios encountered in the plume, these discrepancies have a minimal effect on impingement calculations. The mean free path calculated from continuum results is found to be larger than that found from the direct simulation.

When the direct simulation results at the free-molecular limit are compared to those obtained with the Simons model, the errors are similar to those incurred with the MOC. A difference of 28% is found for impingement quantities.

The divergence of translational and rotational temperature contours, and also axial and radial temperatures, indicates that a large degree of thermal nonequilibrium exists in the flow. Finally, a very small amount of species separation is found in the flowfield, and is explained by the relatively small thermal velocities of the various species. The small degree of species separation experienced shows that it is reasonable to consider the expansion as a homogeneous gas.

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