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Effects of Translational Nonequilibrium on Vacuum Plume Expansions

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The plume flowfield of a helium vent nozzle exhausting into a vacuum is defined by two techniques: the method of characteristics and the direct-simulation Monte Carlo method. The method of characteristics is shown to severely underpredict gas static temperatures due to the assumption of translational equilibrium inherent in the continuum formulation. Mass flow per unit solid angle is shown to be accurately predicted for this flowfield by the method of characteristics until the flow angle approaches within 10 deg of the maximum Prandtl-Meyer expansion angle. Improved treatment of the noncontinuum flow within the nozzle (near the lip) is postulated to have minor effects on the accuracy of this continuum method in comparison with translational nonequilibrium in the external flowfield. Possible treatment of translational nonequilibrium by the method of characteristics is discussed.

Introduction

THE Infrared Astronomy Satellite (IRAS) has been designed with two liquid helium cryogenic systems and spacecraft attitude control maintained by reaction wheels and magnetic torque coils. Preliminary calculations of torques imposed on the spacecraft due to impingement of vented helium on the spacecraft and statistical effects due to vent manufacturing tolerances indicated that excessive torques could be encountered with the baseline vent system design. Since torques in excess of 2×10^{-4} N-m on any axis exceed the baseline capability of the attitude control system (for which hardware already existed), it was decided to refine the disturbance torque analysis and study options for vent system redesign. A portion of this work involved developing an extremely accurate vent flowfield for use in impingement calculations. This paper presents results of general interest obtained in the development of the flowfield for one of the two vent systems.

The most widely used method for predicting the plume flowfield of a nozzle exhausting into a vacuum is the method of characteristics (MOC).[1] It has been realized for a considerable time that the continuum formulation becomes invalid in highly expanded plumes.[1,2] The direct-simulation Monte Carlo method as formulated by Bird[3] has been successfully applied to noncontinuum flow near the lip of a rocket nozzle[4] and to flow of contaminants into the Space Shuttle cargo bay.[5] However, no direct comparison between the results attained by the MOC and the direct-simulation Monte Carlo method has been attempted.

In view of the very large computer run time[5] associated with the direct-simulation Monte Carlo method, it was felt that a comparison of the results of this method with those of a MOC calculation could be highly useful in defining the limits of the MOC technique and formulating approximate techniques to improve the results obtainable with minimum computer costs.

Analytic Procedure

The computer codes used and their theoretical foundation are well described in the references and will not be detailed herein. The vent flowfield to be described was due to the boil-off of helium in an aperture cover tank that is used to cryosorb contaminants during the first two weeks of the mission. The nominal vent flow rate (through two opposing nozzles) is to be 10 mg/s at separation from the booster. However, attainment of this flow rate is still in some doubt; thus the flow through the nozzles and into space was analyzed for a flow rate of 22.9 mg/s. The nozzle itself consisted of a plug with a conical expansion section machined into it. The inlet tube was approximately 2.54 cm in diameter. The throat of the 15-deg half-angle nozzle was 0.028 cm in diameter and the exit diameter was 0.048 cm.

The flow through the nozzle was analyzed using the Laminar Boundary Layer (LBL) code developed by Back et al. at JPL.[6] The gas total temperature at the entrance to the nozzle was assumed to be equal to the spacecraft shell temperature at insertion of 298 K. This assumption was justified by the fact that the helium (which is a very good thermal diffuser) flows at a very low velocity (approximately 0.1 m/s) through several meters of tubing which has this temperature. A total pressure of 21.8 N/cm^2 was found to correspond to the desired flow rate of 22.9 mg/s.

The LBL program couples a laminar similarity solution for the viscous boundary layer with a one-dimensional isentropic expansion of the inviscid core flow. Although it would have been preferable to obtain a two-dimensional solution for the core flow, the time allotted for this effort did not permit this refinement. The flow angle at the exit plane was assumed to have a conical distribution; zero at the nozzle centerline and 15 deg (the wall half-angle) at the boundary-layer edge. This should introduce only small errors and will not affect the comparison of plume expansion techniques in any event. At the exit plane the core flow was found to have a Mach number of 2.703, and 16.4% of the flow was contained in the boundary layer.

It has been noted by Bird[2,4] and Seubold[7] that in the vicinity of the nozzle lip the no-slip boundary condition at the nozzle wall breaks down. Using the direct-simulation Monte Carlo technique, Bird has shown[2,4] that the Mach number at the wall rises to unity at the exit plane and that the flow angle may significantly exceed the nozzle wall angle. To account for these effects, a direct-simulation Monte Carlo analysis was conducted of the flow near the lip of the helium vent nozzle. The axisymmetric computer code used was developed by McGregor[8] for application to rocket plume expansion and impingement. The analysis was confined to a rectangular region starting one boundary-layer thickness (using the exit plane boundary-layer velocity thickness predicted by the LBL code) inside the nozzle. The lower radial boundary was located at the edge of the boundary layer (as predicted by the

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LBL code at that point inside the nozzle). This region was divided into 600 cells of uniform dimensions 2.5 μm on a side. The molecule/wall interactions were assumed to exhibit perfect accommodation. Intermolecular collisions were treated by a hard sphere model adjusted for collision energy.[3,8] Seven thousand simulated molecules were used in the flowfield at any one time after steady flow was obtained.

Most of the results noted by Bird in Ref. 2 were obtained, except that the Mach number at the lip was not found to be exactly unity; the computed value was 0.8. It is believed that this was due to the use of the continuum definition of the speed of sound and an overall translational temperature (as opposed to two components of temperature) in a region of strong translational nonequilibrium. The exit plane flow angle was found to be 21.2 deg at the wall, rising to 23.8 deg within a few mean free paths from the wall, and then gradually dropping to 15 deg at the edge of the boundary layer, the latter being consistent with the boundary condition imposed on the core flow. A strong pressure gradient was also found to exist across the boundary layer, with a pressure ratio of 2.5 between the boundary-layer edge and lip. This pressure ratio is the driving force which leads to the increase in flow angle and is a direct consequence of the breakdown of the no-slip condition at the wall.

Attempts to incorporate the exit plane boundary-layer profile derived from the Monte Carlo analysis described above into an MOC expansion beginning at the exit plane were defeated by numerical difficulties encountered with the MOC code. Specifically, the variation of flow angles and pressure near the wall resulted in computation of subsonic Mach numbers. Smith[9] and unpublished work by Seubold[10] indicate that the variable oxidizer/fuel method of characteristics (VOFMOC) computer code[1] may need modification to treat strong pressure gradients across the boundary layer. To avoid these problems, the single-layer replacement method[7] was used to replace the subsonic region of the exit plane boundary layer generated by the LBL code, while conserving the mass flow rate. The VOFMOC code was then used to compute the plume expansion by the method of characteristics. A constant ratio of specific heats of 1.667 was used. This is consistent with a monatomic gas such as helium in translational equilibrium.

A second plume expansion was performed using the direct-simulation Monte Carlo method. The geometry used for this Monte Carlo analysis is shown in Fig. 1. The flowfield was divided into two regions labeled I and II as shown in Fig. 1. Region I, the main region, consisted of 608 cells and had the cell structure shown in Fig. 1. The cell structure shown was selected such that small gradients in macroscopic quantities would occur between adjacent cells near the start line, which had radial dimensions approximately equal to the mean free path. The requirement of the present computer code[8] that the cell structure be defined by a constant cell width in the axial (X) direction and two widths in the radial (R) direction leads invariably to undesirably large cells (significantly larger than the local mean free path) in the dense region near the start line or undesirably small cells (not containing sufficient numbers of molecules for accurate collision calculations) in the rarefied backflow region of the plume. The latter effect was significant in this analysis, as discussed below. Region II consisted of 120 uniform cells. This region was required to treat the strongly noncontinuum flow observed near the lip[2] and extended axially one-quarter exit radius downstream of the exit plane. The lower radial bound of region II was at the edge of the boundary layer and the upper bound was at 1.04 exit radii. Start line 1 was generated from the previous Monte Carlo analysis inside the lip, while start lines 2 and 3 were extracted from the MOC plume. The continuum breakdown criterion of Bird[2,3] indicated that these last two start lines should still lie within the region of valid MOC calculations. Note that the external surface of the nozzle was ignored in this Monte Carlo analysis.

This case was run with 25,000 simulated molecules in the flowfield. It would have been desirable to have a larger sample of molecules, since at the problem boundary the average number of molecules per cell became too low for accurate collisional modeling[3] beyond approximately 70 deg from centerline. This conclusion is based on a requirement of having an average of four or more simulated molecules in each cell when collisions are computed. Unfortunately, cost, computer capability, and time constraints prohibited this refinement. This is not expected to greatly affect the flow density contours since the streamlines have essentially no curvature in the region where collisional modeling breaks down, the boundary of which is described below. However, the calculation of translational temperature (and hence Mach number) from the Monte Carlo data is of questionable validity at large distances from the exit for angles more than 70 deg from the plume centerline.

Results and Discussion

The principal results are expressed in the form of variation of mass flux per unit solid angle and Mach number with angle from centerline at a distance of nine exit radii from the center of the nozzle exit. This is a form commonly used for modeling of far field plumes.[11]

Figure 2 shows the variation of the mass flux per unit solid angle with angle from centerline. The Monte Carlo results are shown with an indication of 3σ statistical scatter that was obtained by taking the standard deviation of the mean over the last 25 flowfield samples taken during the Monte Carlo

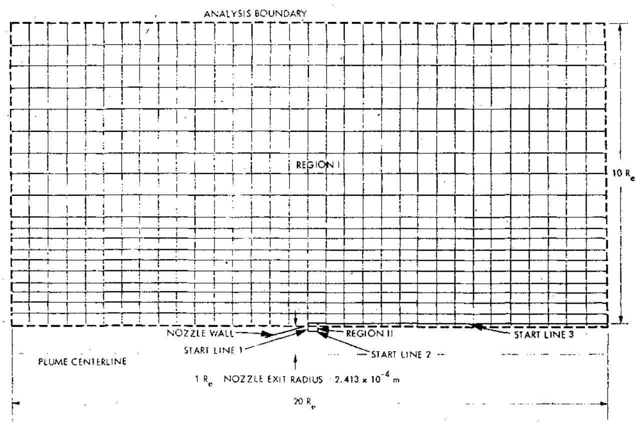

Fig. 1 Monte Carlo plume expansion geometry.

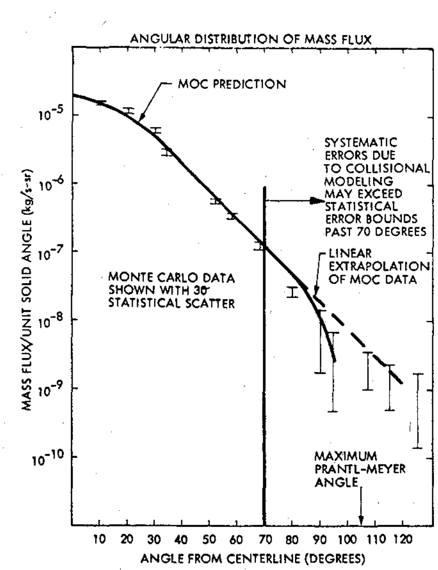

Fig. 2 Angular distribution of mass flux.

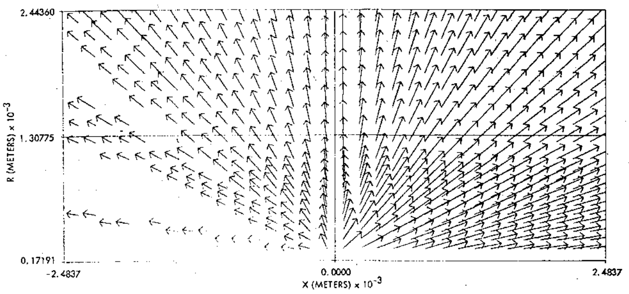

Fig. 3 Velocity field predicted by Monte Carlo.

run after steady-state conditions were achieved. It can be seen that there is no highly significant variation between the MOC and Monte Carlo results until the angle from centerline exceeds 90 deg. Although the maximum Prandtl-Meyer angle for continuum flow would, in this case, be 105 deg (based on Mach 1 flow parallel to the nozzle wall), the VOFMOC code generated no points beyond 95 deg due to the numerical difficulties of expanding completely to a vacuum.[1] The previously mentioned breakdown of collisional modeling by the Monte Carlo method at large angles from the plume centerline is not expected to affect this result materially until the flow angle exceeds 125 deg. This is motivated by the straight streamlines and good convergence of velocity beyond this angle shown in Fig. 3. However, the systematic errors introduced by collisional modeling at large angles may invalidate the error bounds shown beyond 70 deg from centerline. Between 90 and 125 deg the Monte Carlo results show the approximate linear decrease of the logarithm of mass flux per unit solid angle with angle from centerline which is often noted in test data[12] of rocket engines near and beyond the maximum Prandtl-Meyer angle.

The MOC results for the logarithm of mass flux per unit solid angle have a distinct linear variation with angle from centerline prior to becoming steeper approximately 20 deg from the maximum Prandtl-Meyer expansion angle. The linear extrapolation of this region shown in Fig. 2 provides a conservative envelope for the Monte Carlo results. Although the results of one special case are not sufficient to draw general conclusions, this may indicate a method of obtaining a conservative, yet reasonable, plot of mass flux per unit solid angle from the VOFMOC computer code. Care must be used when extending this concept to the gas mixtures encountered in rocket engine plumes, however, as molecular diffusion of light species into the backflow will occur[2,13] and may significantly distort the mass flux curve.

Finally, it should be noted that the breakdown in the MOC results appears to occur near the maximum Prandtl-Meyer angle. Including the larger exit plane flow angles predicted by the Monte Carlo analysis of the lip region would shift this breakdown less than 10 deg and might not substantially increase the large-angle accuracy of the MOC. However, this will require further investigation, although, as discussed above, the definition of continuum properties such as Mach number becomes difficult in this region of noncontinuum flow.

Figure 4 shows the variation of Mach number at a distance of nine exit radii from the nozzle exit with angle from centerline. As before, the Monte Carlo results (which were computed from the overall temperature) are shown with an indication of statistical scatter. In this case, the breakdown of collisional modeling beyond 70 deg in the Monte Carlo analysis is certain to be significant so no data are presented beyond this angle. However, statistically significant differences between the two methods begin to appear before 20 deg from centerline. The MOC results overpredict the Mach number due to underprediction of the translational temperature as shown in Fig. 5, where the isothermal contours for 10 K are shown along with the boundary of accurate

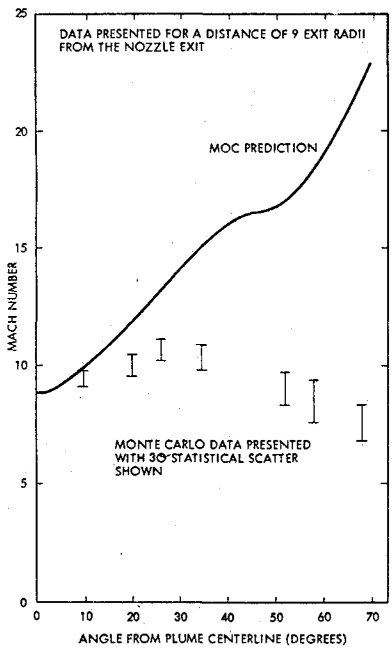

Fig. 4 Mach numbers vs angle from centerline.

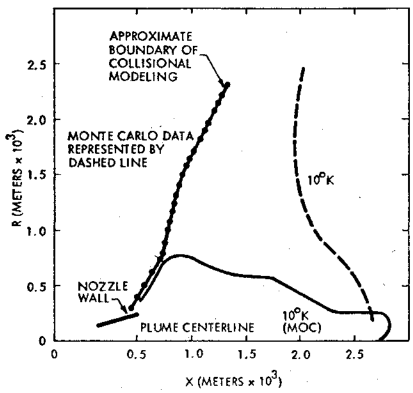

Fig. 5 Constant temperature contours.

collisional modeling. This is an expected result, as Bird[2] has shown that the breakdown of translational equilibrium can occur at very low angles from the plume centerline. Further, he has shown[2] that the boundary of this transition lies along a streamline in highly expanded regions of the plume. In Fig. 5 it can be seen that agreement between the two techniques breaks down at very low angles from the plume centerline.

These results may be important in several fields of rocket exhaust plume prediction. In contamination studies, local gas temperatures must be known with reasonable accuracy to treat condensation of plume species. The reduced gas velocities associated with higher temperatures may reduce impingement reactions on surfaces immersed in the plume. Finally, plume spectral signatures may be somewhat affected by continuing collisional excitation of rotational and perhaps vibrational modes of polyatomic molecules. Confirmation of these speculations will require careful analysis of a hot rocket exhaust plume containing polyatomic molecules and condensible species.

It may be possible to obtain more accurate modeling of the temperature using the MOC technique by adjusting the ratio of specific heats upward. However, this adjustment should not be correlated with Mach number, since the flow along the centerline has been predicted[2] to remain in equilibrium. It may be most productive to correlate the ratio of specific heats with the breakdown parameter[2] (which reflects the degree of translational nonequilibrium)

$$P = \frac{q}{\rho \nu} \frac{\partial \rho}{\partial s}$$

where q is the flow speed, ρ the gas density, ν the collision frequency, and s the distance along a streamline. A correlation of this type may vary for the different gases found in a rocket plume. If such a correlation cannot be formulated theoretically, a one-dimensional Monte Carlo analysis could perhaps be used as a tool for numerical experiments to allow extraction of "empirical" relations.

Conclusions and Recommendations

The method of characteristics has been shown to give an accurate estimate of mass flux per unit solid angle until quite close to the maximum Prandtl-Meyer expansion angle. It may be tentatively postulated that extrapolation of the linear portion of this curve may give reasonable and conservative estimates of mass flux beyond the limiting streamline.

The method of characteristics has been shown to severely underpredict translational temperatures due to the onset of translational nonequilibrium. An engineering solution to this problem may be to correlate an upward adjustment of the ratio of specific heats with the breakdown criterion proposed by Bird.[2] Alternately, a more conventional molecular relaxation scheme could be implemented.

More work in this area may be significant in the fields of plume contamination, impingement, and radiation. The analysis of a case for which there are test data available for comparison is clearly needed. This author feels that the prime candidate for such work is the Aerojet 22.2 N bipropellant thruster tested extensively at AEDC.[12] Another possible subject is the MBB 10 N thruster being used on the Galileo spacecraft. However, important improvements in the present direct-simulation Monte Carlo computer code should be made to limit requirements on computer resources. The present analysis consumed 6 h of central processing unit time on a Univac 1100/81 and required 245K (decimal) words of memory. These requirements could be reduced drastically (perhaps by an order of magnitude) and computational accuracy increased by employing a more flexible cell structure than that used in the present code. The author feels it would be very effective to implement adaptive grid techniques analogous to those used in other numerical fluid dynamics computer codes, possibly in conjunction with the multiple restart method proposed by Chirivella.[14]

Finally, an attempt should be made to implement an engineering solution to the method of characteristics. This would probably require numerical experiments using the direct-simulation Monte Carlo method, but then could perhaps approximate those results at much lower computing costs. However, it is likely that the direct-simulation Monte Carlo method will continue to be required for accurate calculation of noncontinuum impingement effects on surfaces immersed in rocket exhausts such as on the Galileo spacecraft.[13] Further, in cases (such as contamination studies) where molecular diffusion of gas species is important, the Monte Carlo technique is likely to remain the state-of-the-art. These considerations provide strong justification for efforts to improve the computational efficiency of this method.

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