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DIRECT SIMULATION OF EFFUSION AND EXPANSION FLOWS FROM A SLIT INTO A VACUUM

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Abstract

Effusion flows from a two-dimensional porous surface and expansion flows from a sonic slit were studied based upon the DSMC method. Present simulation was carried out under the suspicion that thermal motion of gas molecules would partially change into back flow in effusion flow. Effusion flow was accelerated to a supersonic expansion flow but the virtual stagnation pressure of this expansion flow was much lower than the pressure at the surface. Features of effusion flow with back flow were revealed. No substantial back flow was seen even in the effusion flow from a porous surface. The back flow seemed to be separated from the main flow of the effusion and effects of the back flow were very restricted. Several cell sizes were employed in the simulation of expansion flow. It was found that cell size should be finer than (slit hight/60) × (slit hight/60) so that we might obtain accurate density contour. Value of the parameter $p_0 d$ used in the simulation was about 24torr-mm, which was comparable with the conventional experimental conditions.

1. Introduction

The space is the huge sink of molecules. Because of the low external pressures encounters, gases expand from any sources and form huge jet plumes in which continuum to free molecular flows are included. Jets exhausting from control nozzles of spacecrafts are the representative sources of such a expansion flow[1),2),3),4),5)]. Evaporation or sublimation of materials from surfaces of space vehicles as well as effusion of remainder of combustion from the nozzle can be a source of such an expansion flow.

Thermal motions of gas molecules exert a flow beyond the Prandtle-Meyer expansion

fan[6]. Thus plume impingement in the direction of the back flow as well as in the direction of the main flow must be taken into account. Such a back flow leads to undesirable effects as contamination, heating, disturbance torque, and inefficient thruster operation[4]. Radiation from gas molecules in the back flow occasionally may become a serious noises for the spectroscopic measurements of the space.

Obtaining laboratory pressure sufficiently low to simulate the space environment is not currently possible, and in the absence of reliable theoretical predictions, numerical simulations based upon direct simulation Monte Carlo (DSMC) method[7] will provides available date for spacecraft engineers and experimentalists of the space materials. As above mentioned, the expansion flows include continuum to free molecular flows. Full scale simulation of the total flow field must be still impossible, and the flow field should be studied separately[8].

In this studies numerical simulations of effusion (exudation) flows from a porous surface of finite width and expansion flows from a sonic slit into a vacuum are carried out. Simulation of effusion flow is intended to know whether or not rest gas expands around a corner considerably. Present simulations cover a rather restricted flow field in the vicinity of the surface or slit. Results obtained by the present simulations can be used as boundary conditions of simulation of far fields in the expansion flow.

Because of simplicity and efficiency of the method, we will apply the Bird's DSMC method[7] based upon the random walk theory rather than the simulation of the Boltzmann equation proposed by Nanbu[9]. It is well known that an appropriate evaluation of the collision rate in each cell is the first requirement in the DSMC method. Two representative time counting technique by Bird[7] and by Koura[10], the null collision technique will be examined in the simulation.

Results of simulation of effusion (exudation) flows will be compared with the kinetic theory analysis of the one-dimensional evaporation problem[11]. This comparison will also reveal that whether or not the effusion flows are analogous to the expansion flows. Results of simulation for expansion flows will be compared with the previous work by Boyd and Stark[12]. Present results will demonstrate detailed features of expansion flows, which will yield undoubtedly more accurate results than the Boyd and Stark's works.

2. Simulation Scheme and Procedure

A. Direct Simulation Monte Carlo Method

Starting from the random walk picture, Kac[13] has proposed for the change of distribution function of N particles (in a microcanonical ensemble) $\phi(\boldsymbol{R};t)$ where $\mathbf{R}$ denotes an array of velocities v_i of N particles instead of Liouville equation, an stochastic equation called the master equation,

$$\frac{\partial \phi}{\partial t} = \sum_{1 \le i < j \le n} \int d\vec{g}\, [\phi(A_{ij}(\vec{g})\boldsymbol{R};t) - \phi(\boldsymbol{R};t)] p_{ij}\,, \tag{1}$$

where

$$A_{ij}(\vec{g})\boldsymbol{R} = \boldsymbol{R}(v_1, v_2, \ldots, v_i', \ldots, v_j', \ldots, v_N)\,,$$

p_{ij} the collision probability of i molecule with j molecule, and v_i' and v_j' are the velocity of i and j molecules after collision, respectively. Kac made two simplifying assumptions; (1) the distribution function depends only on the velocities (or momenta) of the particles, i.e., the master equation describes motions of N particles in a spatially homogeneous gas. (2) the gas is very dilute, so that only binary collisions need to be considered. The transition probability for the random steps can be determined from the dynamics of such a binary collision. The probability of a collision of i molecule of velocity v_i with j molecule of velocity v_j is assumed to be given by Boltzmann's "Stosszahlanzatz".

Kac's master equation Eq. (1) is reduced to the nonlinear Boltzmann equation as $N \to \infty$. Thus numerical simulation of many molecules yields a solution of the Boltzmann equation as sample number $N_{sam} \to \infty$. Dividing the flow field into many cells, assigning N molecules in the cell initially and applying a time increment Δt_m much smaller than mean collision time τ_c, we can execute the motions of molecules step by step. Molecules travel cell to cell through the translational motions, which causes a spatial distribution of molecules. Once we know data of molecules in the cell, we can simulate the collision process after the concept of Kac's. If $\Delta t_m \ll \tau_c$ the first stage of molecular motion (collisionless motion) and the second stage of the molecular motion (collisional process) can be treated separately. This is the idea of simulation originated by Bird[6] called as the DSMC method.

Koura[14] and Beloserkovski and Yanitsky[15] derived simulation schemes based on the Kac's master equation. In the second stage of the simulation the collision probability p_{ij} and sample number of collisions N_a in the interval Δt_m should be determined stochastically. Methods of simulation of Koura[14], Beloserkovski and Yanitsky[15], and Nanbu[9] require evaluation of p_{ij} of the all collision pairs in the cell, so that we must execute a lot of calculation of $O(N^2)$ where N denotes the number of molecules in the cell.

Introducing acceptance-rejection method, Bird reduced this calculation to the order of O(N). The acceptance-rejection method yields the expectation

$$E[\frac{N_{ac}}{N_{tot}}] = \frac{\nu}{\nu_{max}}, \tag{2}$$

where N_{ac} denotes accepted number of collision pairs, $(g\sigma(g))_{av}$ average value of $g\sigma(g)$, N_{tot} the total number of sampled collision pairs, ν the expectation of collisions in the cell in the interval Δt_m given by

$$\nu = \frac{1}{2} N n (g\sigma(g))_{av}, \tag{3}$$

n the number density, g the relative velocity $g_{ij} = |\vec{v}_j - \vec{v}_i|$, σ the collision cross section, and ν_{max} is given by

$$\nu_{max} = \frac{1}{2} N n (g\sigma(g))_{max}. \tag{4}$$

Bird estemated interval of sequent collisions Δt_c by

$$\Delta t_c = \frac{2}{N n (g\sigma(g))_{ac}} \tag{5}$$

where the subscript ac implies the accepted value. The sample number N_{ac} is determined by the following inequalities.

$$\sum_{k=1}^{N_{ac}-1} \Delta t_{ck} < \Delta t_m \leq \sum_{k=1}^{N_{ac}} \Delta t_{ck} . \tag{6}$$

Expectation of Eq. (5) under the condition (6) yields

$$E[\Delta t_c] = \frac{1}{\nu} . \tag{7}$$

This method is called "time counter method". Although the time counter method yields correct (mean) collision rate ν, the sample number N_a is determined by an unstochastical way. For the Maxwell molecules $g\sigma(g)$ is constant with regard to the relative velocity g, so that Δt_c becomes constant.

Since it is natural to consider that occurrence of collisions obeys the Poisson process[16], Δt_c may be determined by the following exponential distribution

$$p(\Delta t_c) = \nu exp(-\nu \Delta t_c) . \tag{8}$$

Equation (8) yields the expectation Eq. (7). Equation (2) is rewritten as

$$E[\frac{N_{ac}}{N_{tot}}] = \frac{\nu \Delta t_m}{\nu_{max} \Delta t_m} . \tag{9}$$

Thus, if $\nu_{max}\Delta t_m$ collision pairs are sampled, expectation of the number of accepted collisions agree with the correct expectation of N_{ac}, $E[N_{ac}]$; substituting Eq. (4) instead of Eq. (3) into Eq. (7), we can obtain the expected sample number $E[N_{ac}]$.

Null collision technique[14] yielded an improvement for the time counting method where $N_{tot} - N_a$ collisions are regarded as null (pseud-) collisions[17]. So long as $N \gg 1$ time counter method yields the same results as the results of null collision technique. In the present simulations both time counting methods are available and they will be employed. As will be shown later, in the simulation of expansion flow from a sonic slit, "time counter method" works well to the extent $N = O(1)$.

B. *Procedure of Simulation*

Monte Carlo simulation of effusion flows from a two dimensional porous surface with and without back flow and expansion flows from a sonic slit are executed in this paper. Since each two-dimensional flow field has a surface of symmetry, the half of the flow field above this surface of symmetry is simulated. This half of the flow field is devided into small cells and N_∞ molecules are initially assigned to each cell where the depth of the cell perpendicular to the two-dimensional plane is taken to be $1 \times \lambda_\infty$ where λ_∞ denotes the mean free path pertinent to the reference state. Setting the cell volume $\alpha\beta\lambda_\infty^3$, we obtain

$$n_\infty \lambda_\infty^3 = N_\infty / \alpha\beta , \tag{10}$$

where n_∞ denotes the number density of reference state. Equation (10) yields the relation

between the number density of simulated molecules N_∞ and the number density of real gas n_∞.

Boundaries of the flow field of simulation are solid wall, edges of simulated domain in the flow field, and a porous surface or a slit of the width D. For each boundary we employ the following (a) to (d) boundary conditions.

(a) **Porous surface or sonic slit:** One additional array of cells are provided and number of molecules in the cell is remained constant. Velocities of gas molecules obey Maxwellian distribution pertinent to a stagnation condition or to a sonic condition. The stagnation condition is given by pressure $p = p_0$, temperature $T = T_0$, and number density $n = n_0$. The sonic condition is given by pressure $p = p^*$, temperature $T = T^*$, number density $n = n^*$, and velocity $u = (\gamma R^* T^*)^{1/2}$ where γ is the ratio of specific heats and R* is the gas constant. Molecules move to the next cell in the simulated domain by random walks.

(b) **Solid wall:** Molecules impinged on the solid wall pararell to the porous surface or to the slit suffer specular reflection, while molecules impinged on the wall perpendiculat to the porous surface suffer diffuse reflection.

(c) **Surface of symmetry:** Molecules impinge on the surface of symmetry reflect specularly.

(d) **edges of the simulated domain:** These boundaries act as molecular sinks, i.e., no molecules enters into the simulated domain through these surfaces.

Initially 10 or 5 molecules are fed in the all cells in the domain of simulation. We assume that temperature of solid wall is same as the temperature of stagnant gas. Under these initial and boundary conditions, molecular motions are simulated with the aid of the DSMC method. Simulation is executed employing hard sphere molecules.

In the case of effusion flows the initial pressure ratio is set $p_0(0)/p_\infty(0) = 8$ and the half-height $(D/2)$ of the porous surface is set $5\lambda_\infty$ to $20\lambda_\infty$ for the simulation of flow field; mean free path λ_0 of the rest gas for this pressure ratio is given by $\lambda_0 = \lambda_\infty/8$ and the corresponding Knudsen numbers $\mathrm{Kn}_0 = \lambda_0/D$ are in the range from 0.0125 to 0.003. The cell size is changed from $0.2\lambda_\infty \times 0.2\lambda_\infty$ to $1.0\lambda_\infty \times 1.0\lambda_\infty$. The simulated flow domains are shown in figures shown later. In order to obtain an asymptotic value of sonic point simulations for small values of Knudsen number are also carried out.

In the case of expansion flows from a sonic slit initial pressure ratio is set $p^*(0)/p_\infty(0) = 8$ and the height of the slit is set $30\lambda_\infty$. The Knudsen number pertinent to the sonic condition is $\mathrm{Kn}^* = 0.004$. Cell size is changed from $0.1\lambda_\infty \times 0.1\lambda_\infty$ to $1.0\lambda_\infty \times 1.0\lambda_\infty$. Simulated flow domain is $40\lambda_\infty \times 100\lambda_\infty$.

3. Results and Discussion

Direct simulations of three flow configurations were carried out; i) effusion flow without back flow, ii) effusion flow with back flow, iii) expansion flows from a sonic slit. Sampling numbers and CPU times of representative cases are shown in Table 1. Several cell sizes were employed in the simulation. Present results suggested that the half width of the slit should be divided (at least) into about 30 cells. For the case of $\mathrm{Kn}* = 0.004$ a cell size $0.5\lambda_\infty \times 0.5\lambda_\infty$

was small enough to simulate expansion flows from a sonic slit. A preferable cell size was thus dependent upon the Knudsen number Kn*. But for the simulation of Knudsen layer in the effusion flow this cell size was apparently insufficient and a finer cell may be occasionally necessary for the detailed analysis.

Table 1: Values of parameters used in the simulations

flow	method	molecules/cell	sampling number	cpu time (minute)
effusion without backflow	NC	5	12500	170 ($d = 40\lambda_\infty$)
effusion with backflow	TC	5	12500	9
	NC	5	12500	11
expansion flow	TC	10	7500	120
	NC	10	7500	140

i) Effusion flow without back flow.

In Fig. 1 present results for $D = 40\lambda_\infty$ (temperature, density, and pressure along the line of symmetry) are compared with the results of one-dimensional evaporation problem[11]. Asymptotic values as $x \to \infty$ of temperature, number density, and pressure of the one-dimensional evaporation problem were 0.640, 0.326, and 0.209, respectively. Since the Knudsen number $\mathrm{Kn}_0 = \lambda_0/D$; $\lambda_\infty = 8\lambda_0$ was not so small, no quasi-onedimensional effusion flow was established adjacent to the porous surface and features of two-dimensionality were shown in the vicinity of the Knudsen layer.

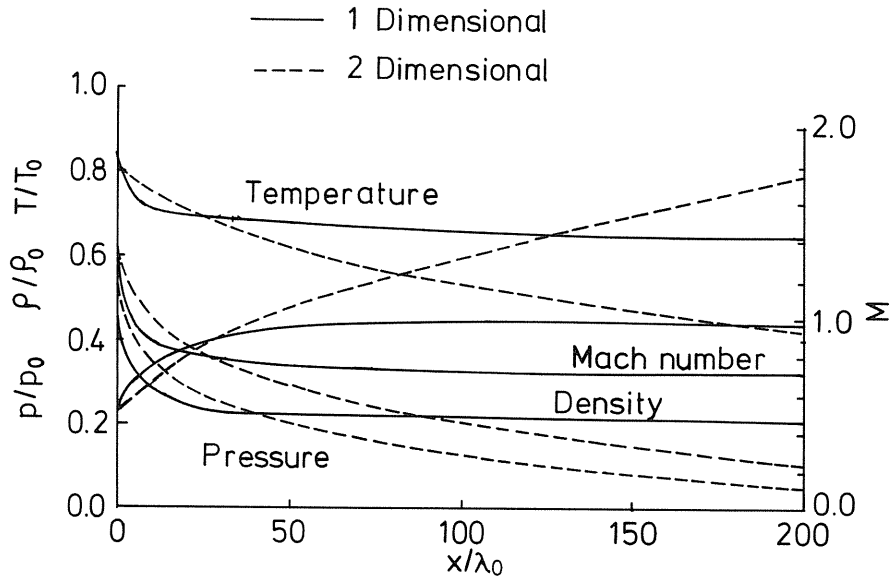

Fig. 1. Comparison of two-dimensional effusion flow with the one-dimensional evaporation flow: Distributions of number density, pressure, temperature, and Mach number along the line of symmetry.

In Fig. 2 location of the sonic line x_s/D on the symmetric line $y = 0$ (or surface) in the effusion flow was plotted vs reciprocal of the Knudsen number Kn_0 The results shown in Fig. 2 were obtained employing large cell sizes like a $5\lambda_\infty \times 5\lambda_\infty$ as well as small cell sizes. Present results showed that the distance tended to approach a finite value, say $x_s/d \approx 0.11$, and $p/p_0(x_s) \approx 0.21$.

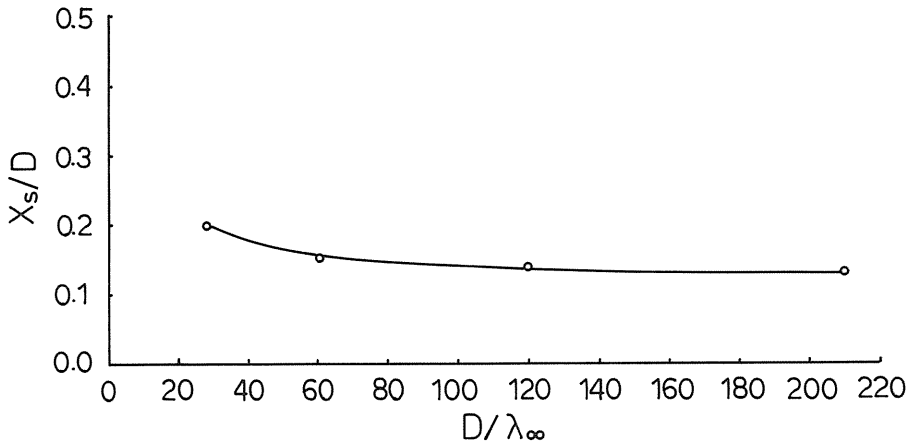

Fig. 2. Location of the sonic point along the line of symmetry vs reciprocal of the Knudsen number D/λ_∞.

This result suggests that the effusion flow from a two-dimensional slit is rapidly accelerated in the vicinity of the surface up to the sonic velocity. Thereafter a supersonic expansion flow is established. As the Knudsen number decreases, this sonic condition of the effusion flow may approache the sonic condition of the one dimensional evaporation flow except the region in the vicinity of edges of slit.

Thus the effusion flow into a vacuum may be equivalent to an expansion flow from sonic slit located at $x_s/D \approx 0.11$. Stagnation condition of this equivalent expansion flow becomes

$$\begin{aligned} T_{0eq} &= 0.64(\gamma/2)\, T_0 \,, \\ p_{0eq} &= 0{,}21(\gamma/2)^{\frac{\gamma}{\gamma-1}} p_0 \end{aligned} \tag{11}$$

for the moatomic gas ($\gamma = 5/3$). But we need further simulations to assert whether or not $x_s/D = 0.11$ is true in the three dimensional flow.

ii) effusion flows with back flow;

In Figs. 3 to 5 were shown results of simulation with null collision technique of the effusion flow with back flows. Velocity vectors in the simulated domain were shown in Fig. 3. It was very interesting that the backflow was separated by a flow parallel to the slit surface (see Fig. 3). It was apparent that most part of the expansion flow was not affected by the back step and a small portion of the expansion flow in the vicinity of the edge of the slit contributed to the back flow. Figure 4 showed density contour (ρ/ρ_0) in the simulated domain.

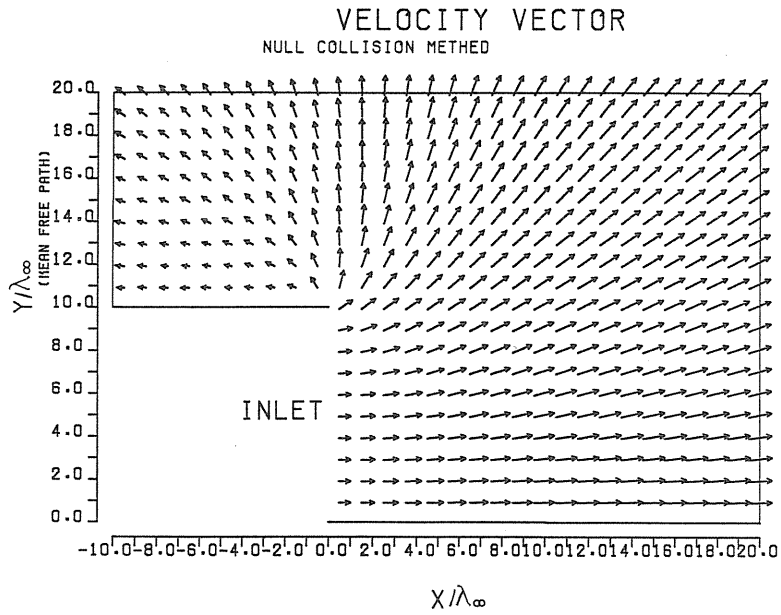

Fig. 3. Velocity vectors in the effusion flow with back flow taken from the simulation employing the null collisionn tecknique; Kn* = 0.006.

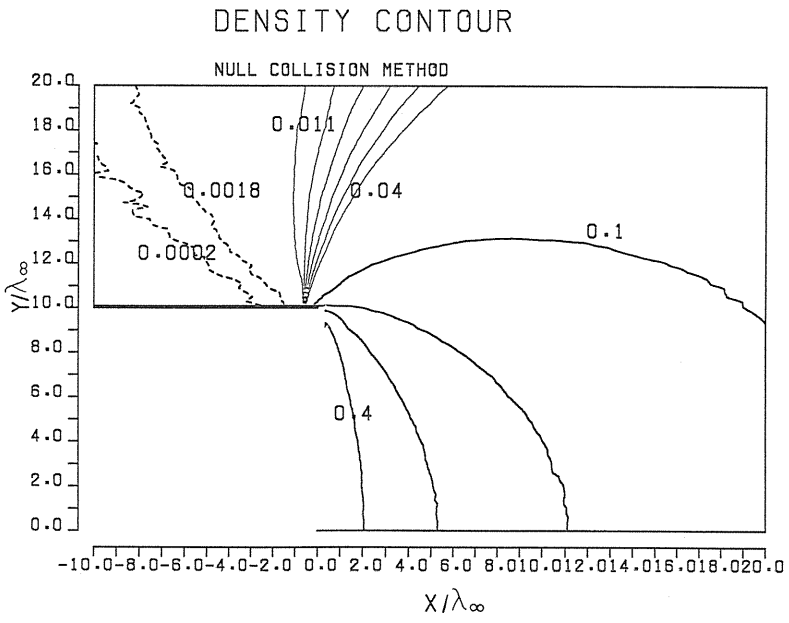

Fig. 4. Density contour in the effusion flow with back flow taken from the simulation employing the null collisionn tecknique; Kn* = 0.006.

Since the number density was proportional to the average number of molecules in the cell N_{av}, $\rho/\rho_0 < 0.01$ was corresponding to $N_{av} < 1$ in the present simulation. Nevertheless, time average (average of many samples) of density yielded unambiguous contours unexpectedly. Simulations with time counter method also yielded accurate density contours even for the case $N_{av} \approx 0.5$, so long as the present problem was concerned.

As was shown in Fig. 4, expansion fan around the corner (edge of the slit) was very weak. Knudsen number on the contour, $\rho/\rho_0 = 0.01$ was estimated as $Kn = (1/40 \times 8)/(\rho/\rho_0) \approx 0.3$, i.e., the expansion fan was a flow in the transition regime. Thus, as was shown in Fig. 5, expansion flow was not so accelerated behind the slit; roughly speaking iso-Mach lines were parallel to the slit. But this fact did not mean that effects of collisions in this region were not important. The directions of velocity vector were widely changed through this expansion fan (see Fig. 3).

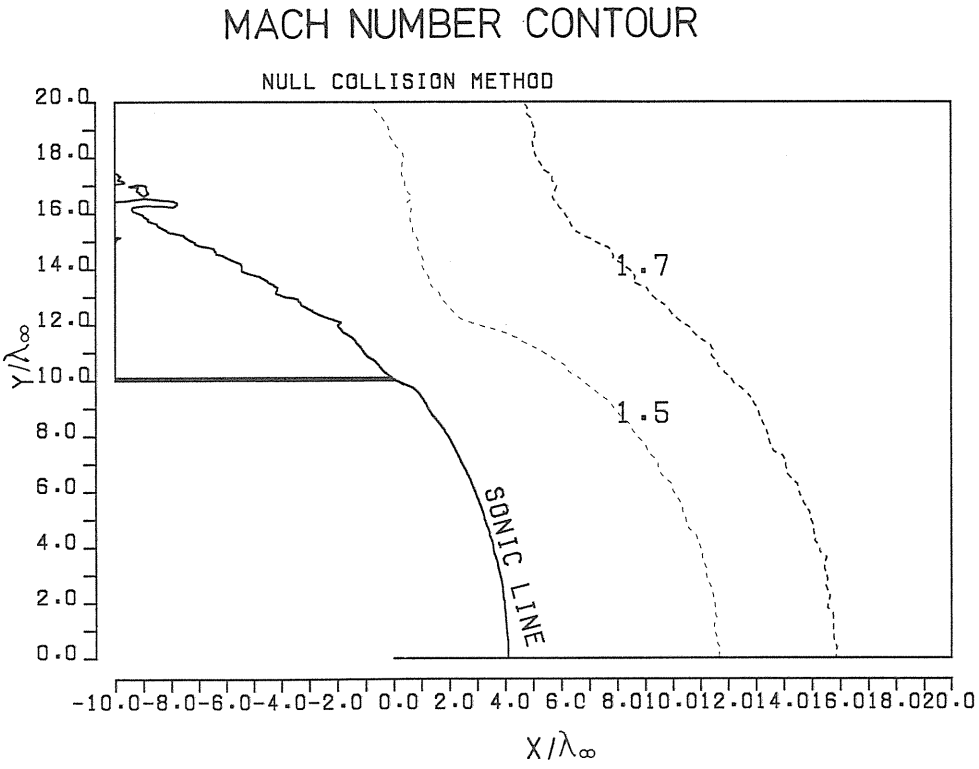

Fig. 5. Mach number contour in the effusion flow with back flow taken from the simulation employing the null collisionn tecknique; Kn* = 0.006.

The results using the null collision technique yielded a little smaller density predictions than the results obtained by use of the time-counter method; the null collision technique rather than the time-counter method yielded slightly rapid expansion.

iii) Expansion flow from a sonic slit

In Figs. 6 and 7 were shown density contours of expansion flow from a sonic slit taken from numerical simulation employing the null collision technique and the time counter method, respectively. Molecular numbers per cells was 10 in the simulations. Results of the time counter method yielded almost same results as those which the null collision technique yielded.

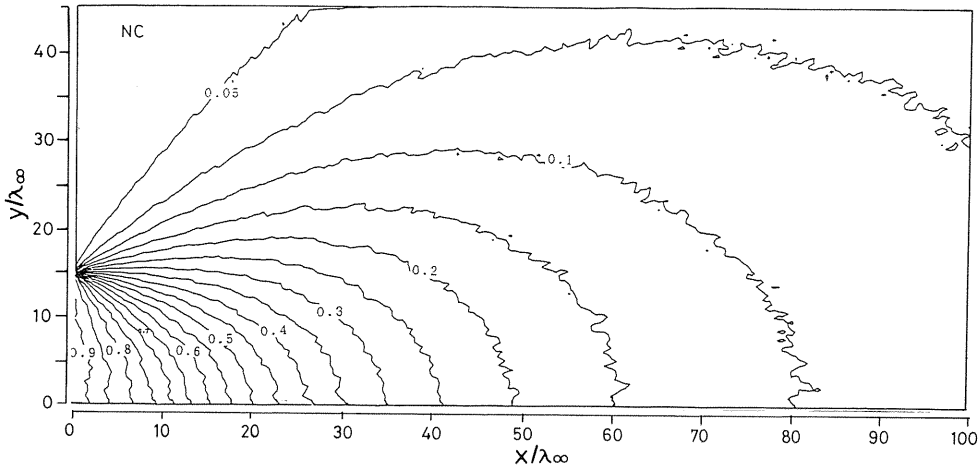

Fig. 6. Density contour in the expansion flow from a sonic slit taken from the simulation employing the null collisionn tecknique; Kn* = 0.004.

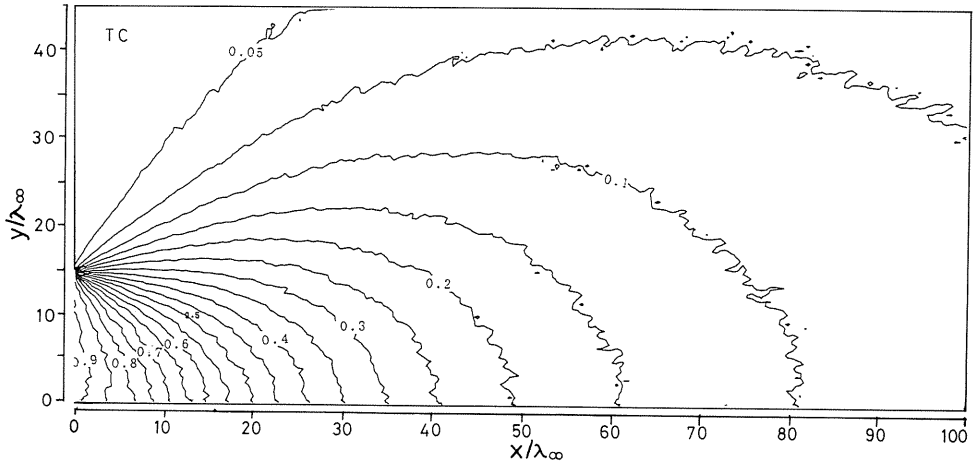

Fig. 7. Density contour in the expansion flow from a sonic slit taken from the simulation employing the time counter method; Kn* = 0.004.

Boyd and Stark[12] carried out a simulation of expansion flow from a sonic slit for Kn* = 0.03. Figures 8 and 9 showed density contour and velocity vectors taken from the present simulation employing null collision technique for Kn* = 0.03. Cell size employed was $1.5\lambda^*$ $\times$ $0.5\lambda^*$. Even if we employed a large cell size $5\lambda^*$ $\times$ $3\lambda^*$ which Boyd and Stark employed present results showed a quantitative disagreement with the results of Boyd and Stark (see Fig. 1 in reference 12).

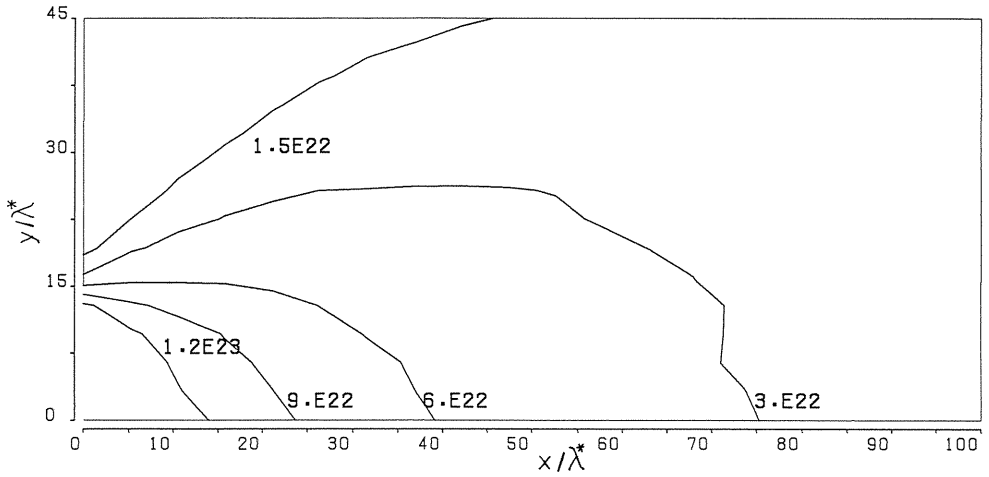

Fig. 8. Density contour in the expansion flow from a sonic slit taken from the simulation employing the null collision technique; Kn* = 0.03.

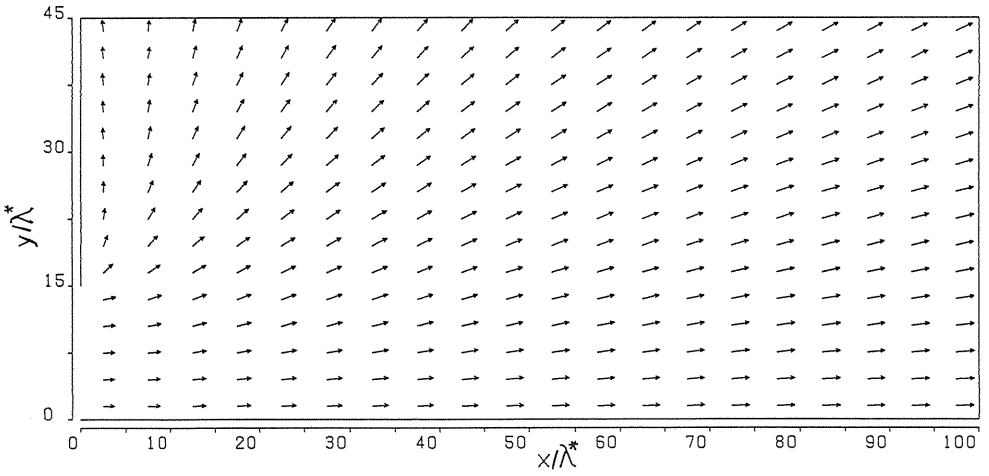

Fig. 9. Velocity vectors in the expansion flow from a sonic slit taken from the simulation employing the null collision technique; Kn* = 0.03.

So far as number density is concerned the present results for $x/D \geq 1$ agree with the solution of Euler equation. The expansion flow along the line of symmetry (surface of symmetry) approached a cylindrical expansion flow from a virtual line source.

Since the present simulation, in the dimensional expressions, is equivalent to an expansion of gas with stagnation pressure $p_0 = 3.2$kPa from a slit 1mm in height (i.e., $p_0 d = 24$torr · mm) into a vacuum; this value of the parameter is in the range of conventional experiments. A detailed comparison of the present results with experimental results will yield useful informations on the DSMC method.

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