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DIRECT MONTE CARLO SIMULATION OF AXISYMMETRIC FREE JET

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Abstract

Axisymmetric expansion flow from a circular orifice into a vacuum was studied based upon the DSMC method. The numerical simulation was carried out for the gas composed of the hard sphere molecules. It is found that the radial temperature is slightly higher than the axial temperature in the vicinity of the orifice. The degree of such a nonequilibrium decreased in accordance with the decrease of the Knudsen number Kn. For the case of Kn = 0.02 the difference between two temperatures was less than 2%. Present simulation revealed that in the vicinity of the axis of symmetry orifice flow expands like a spherical source flow but the off axis flow exhibites the peculiar features of axisymmetric expansion flow predicted by Grundy. The simulated expansion flow along the axis of symmetry includes continuum to free molecular flows. Present results, the terminal velocity, the terminal temperature, and the terminal Mach number, showed a good agreement with the previous results of spherical source flow expansion.

1. Introduction

Expansions of free jets into a vacuum or into a low ambient gas were studied intensively in 50 to 60 decades in accordance with the development of space explorations. The free expansion flow was used as a low density and hypersonic flow[1] as well as for the studies of plume impingement and contaminations of space vehicles and instruments. In the next decades studies on the free jet and molecular beam were spreaded further because the surface science is substantialy important for the production of semiconductors.

Molecular beams produced by skimmers and collimators were analyzed by the time-of-flight technique[2]. Theoretical prediction of the velocity distribution function and/or

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temperatures in the free jet was a counterpart of this experiment. Hamel and Willis[3] and Edwards and Cheng[4] studied spherical source flow expansion so that they might obtain the expansion flow along the axis of free jet. They yielded analytical solutions of the terminal temperature using the hypersonic assumption. Chen[5] and one of the present author[6),7] studied the same proble for the case of finite source Knudsen number Kn_D. Grundy[8] treated axially symmetric free jet whose solution is valid in the core around the axis of symmetry. Results of Grundy showed that off axis temperature is higher than the temperature on the axis for $x/D > 0.1/Kn$, which is a distinctive feature of the expansion of the axisymmetric free jet.

In the experiments of underexpanded free jet flow properties along the axis of symmetry are usually measured and off axial diagnoses are scarecely carried out. So, the Grundy's prediction on the radial distribution of temperature might be remained unconfirmed experimentally. Direct simulation using the Monte Carlo method (DSMC)[9] is a numerical experiment of physical phenomena as far as molecular dynamics and boundary conditions are physically acceptable. Bird[10] carried out DSMC experiments of spherical source flow expansions. Many DSMC experiments of free jet expansions from an orifice or a supersonic nozzle were presented but investigations of thermal nonequilibrium in the expansion flow are not attacked till now.

In this note DSMC experiment of expansion of axisymmetric free jet into a vacuum are carried out. Present simulation is intended to reveal the thermal nonequilibrium in the off axis region as well as along the axis of symmetry in the expansion flow. Because of simplicity and efficiency of the method, Bird's DSMC method[9] based upon the random walk theory is employed rather than the method proposed by Nanbu[11]. In order to count collisional interval Koura's[12] null collision (NC) technique is used.

2. Simulation Procedure

Monte Carlo simulation of expansion flows from a sonic orifice into a vacuum is executed in this paper. Axisymmetric flow field of the expansion flow is divided into coaxial annular disks (cells) with the thickness Δz and the width Δr where the radius of the inner and the outer cylinders are $(N-1) \times \Delta r$ and $N \times \Delta r$, respectively. A schematic drawing of the calculation domain, $r_{max} = 2D$ and $z_{max} = 10D$, is shown in Fig. 1 where the plane, $z = 0$ perpendicular to the axis is on the sonic orifice and D denotes the diameter of the orifice. Three dimensional motions of molecules in each cell are projected on a rectangular (two-dimensional) plane, $(N-1) \times \Delta r \leq r \leq N \times \Delta r$ and $(M-1) \times \Delta z \leq z \leq M \times \Delta z$. A molecule having a velocity $v = (v_r, V_\theta, v_z)$ and a position (r, z) at time t shifts to (r′, z′) where

$$r' = [(r + v_r \Delta t)^2 + (v_\theta \Delta t)^2]^{1/2},$$

$$z' = z + v_z \Delta t$$

at $t = t + \Delta t$. Molecular velocity (v'_r, v'_θ, v'_z) at (r′, z′) is given by

$$v'_r = [v_r(r + v_r \Delta t) + v_\theta v_\theta \Delta t]/r',$$

$$v'_z = v_z,$$

$$v'_\theta = [v_\theta(r + v_r \Delta t) - v_r v_\theta \Delta t]/r'$$

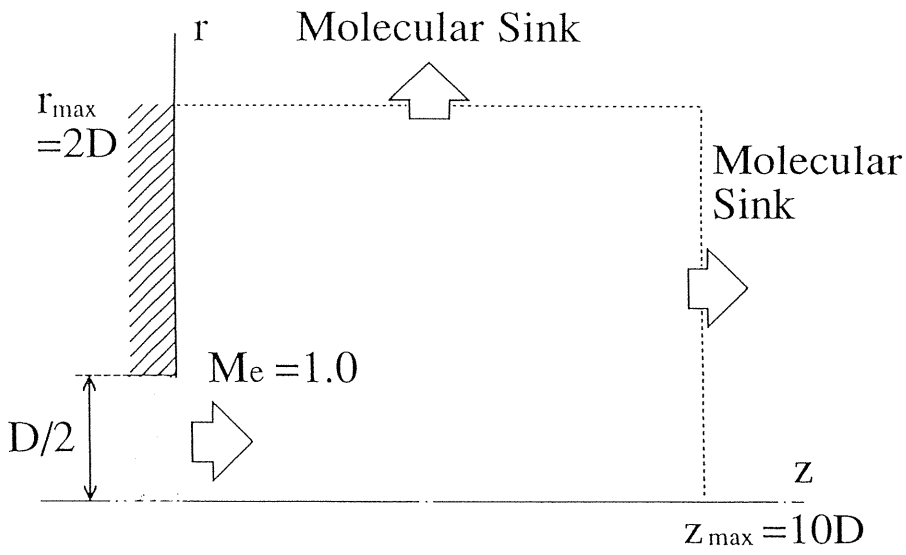

Fig. 1. Domain of numerical simulation of orifice flow.

Molecules pass through the axis of symmetry are, thus, suffer specular reflection at $r=0$ on the two-dimensional plane. Molecules are supplied through additional cells just inside the orifice. The number of molecules feeded in the smallest cell including the nozzle axis is no less than 10. Boundaries of the calculation region are a sonic orifice of the radius r = D/2, a solid wall, the symmetric axis of the expansion flow, and boundaries of the simulated domain in the flow field (See Fig. 1). For each boundary the following (a) to (d) boundary conditions are employed.

(a) **Sonic orifice:** One additional array of cells of $1\times\lambda^*$ thickness are provided inside the orifice. The number of molecules fed in each additional cell is kept constant and velocities of the molecules in the cells obey Maxwellian distribution pertinent to the sonic conditions: It is assumed that molecules enter into these cells through the orifice are instantaneously equilibrated with ambient gas, i.e., these molecules are changed with new molecules obeying to the Maxwellian distribution. The sonic conditions are given by pressure $p=p^*$, temperature $T=T^*$, number density $n=n^*$, velocity $u=(\gamma RT^*)^{1/2}$, γ, 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 impinging on the solid wall parallel to the orifice suffer specular reflection,

(c) **Symmetric axis:** Molecules impinging on the symmetric axis reflect specularly.

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

Number of molecules in the cell is precisely proportional to the volume of the cell and the molecules in the additional cells ($x\leq 0$) are homogeneously distributed in the space. Location of the molecules are stocastically determined using random number R_{an}: $r=r_{max}\times(R_{an})^{1/2}$. The all cells in the simulation region are initially empty, i.e., vacuum.

3. Results and Discussion

Simulations were carried out using the hard sphere molecules for various values of the Knudsen number. The smallest value of the Knudsen number applied was 0.02. Since, in the pleriminary study, results of simulation for $r_{max}=2D$ yielded the same results as the ones for $r_{max}=3D$, we employed $r_{max}=2D$ in the present simulation. On the other hand, a uniform cell size, $\Delta z=1\times\lambda^*$ and $\Delta r=1\times\lambda^*$ was employed. So, the maximum size of the simulation domain was $100\lambda^*\times500\lambda^*$ for $\mathrm{Kn}=\lambda^*/D=0.02$. The time increment Δt_m of collisional process and collisionless motion of molecules was set as $\Delta t_m=\tau_c^*/10$ where τ_c^* is the mean free time defined by $\lambda^*/(2RT^*)^{1/2}$. Usually, sampling interval N_{sam} is chosen as $N_{sam}\geq[(\tau_c)_{loc}/\Delta t_m]_{max}$ where $(\tau_c)_{loc}$ denotes the local mean free time. Since, in the expansion flow, the local mean free time increases as the expansion proceeds, the abovementioned definition of the sampling interval becomes inconvenient. But the previous study[13] on the hypersonic flow suggested that the time interval $\Delta t=2\Delta x/U$ where Δx denotes the cell width in the flow direction and U denotes the flow velocity is sufficient to realize uncorelated collisional process in the original cell. So, the following sampling interval is employed;

$$N_{sam}=Max\{[(\tau_c)_{loc})/\Delta t_m]_{min},\ (2\Delta z/U)_{max}\}$$

For $\mathrm{Kn}=0.02$ sample molecules in the simulation domain were about 1.8×10^6 and the sampling times were 1.0×10^4.

In Figs. 2 and 3 are shown number density contours of expansion flow from a sonic orifice for $\mathrm{Kn}=0.1$ and 0.02, respectively. The contour for $\mathrm{Kn}=0.1$ is almost same as the contour for $\mathrm{Kn}=0.02$. But thermal motions of molecules in the direction of $z(T_z)$, $r(T_r)$, and $\theta(T_\theta)$ are not in thermal equilibrium. A degree of nonequilibrium $(T_r-T_z)/T_r$ is presented in Fig. 4. If the orifice is so small as $D=50\lambda^*$, viscous effects will take place in the actual expansion flow. So, the velocity distribution function of gas molecules will be given as Navier-Stokes or Chapmann-Enskog distribution. In the present simulation we ignore a slight (about 2%) nonequilibrium in the vicinity of the orifice shown in Fig. 4.

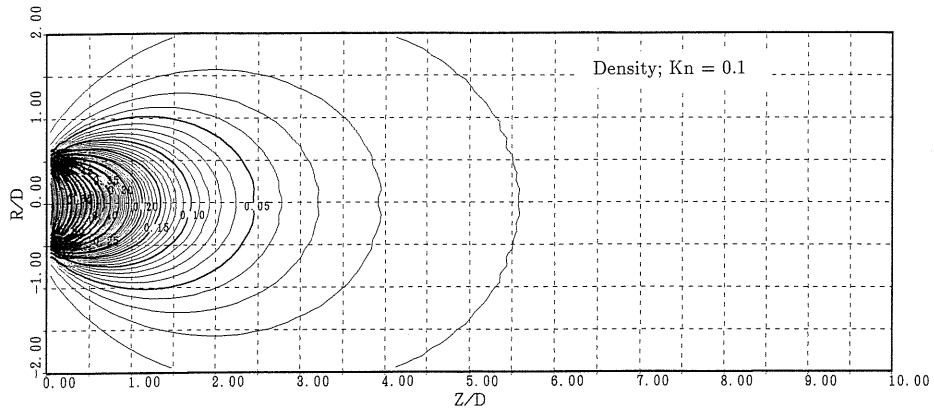

Fig. 2. Number density contour; $Kn=0.1$.

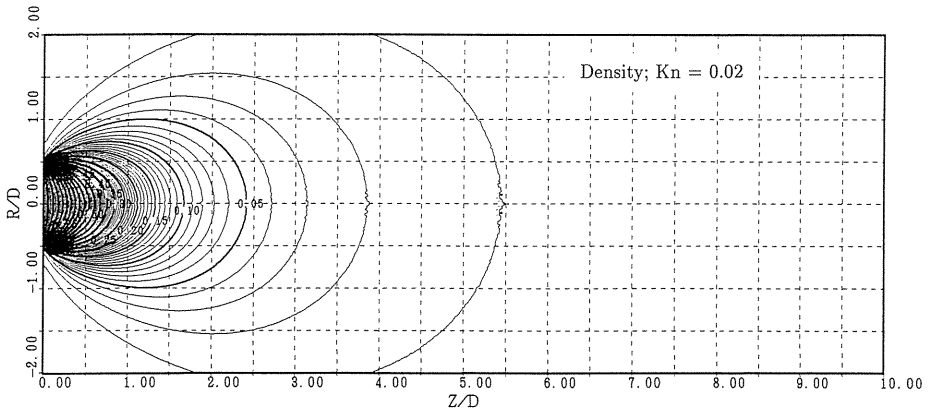

Fig. 3. Number density contour; $Kn = 0.02$.

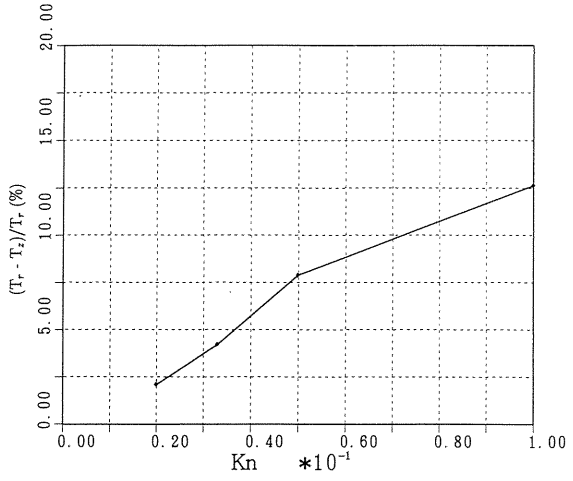

Fig. 4. Degree of nonequilibrium, $(T_r - T_z)/T_r$ in the vicinity of the orifice vs Kn.

The stream line, i.e., Mass flow rate is shown in Fig. 5. The region adjacent to the wall parallel to the orifice is almost vacuum: Since the inclination of the line for $m_{flux} = 1$ is about 80° from the z axis, the continuum theory yields $p = 3 \times 10^{-5} p^*$ on this line. Velocity vectors and contour of Mach number are presented in Fig. 6. Since molecules impinged on the wall parallel to the orifice reflect specularly, expansion flow slips on the wall. The contours of Mach number in the vicinity of the axis sugget that the axisymmetric free jet expands like a source flow. But, as is shown in the figure, curvature of the contour decreases as the expansion proceeds. Eventually, the curvature becomes negative, i.e., we find the concaved contour for $z/D \geq 5$. This criterior implies $z/D \geq 0.1/\mathrm{Kn}$[8].

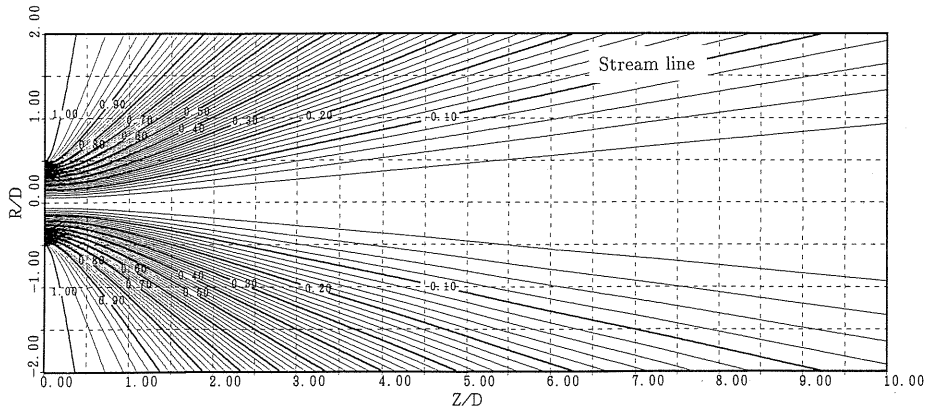

Fig. 5. Contour of constant mass flux (stream line); $Kn=0.02$.

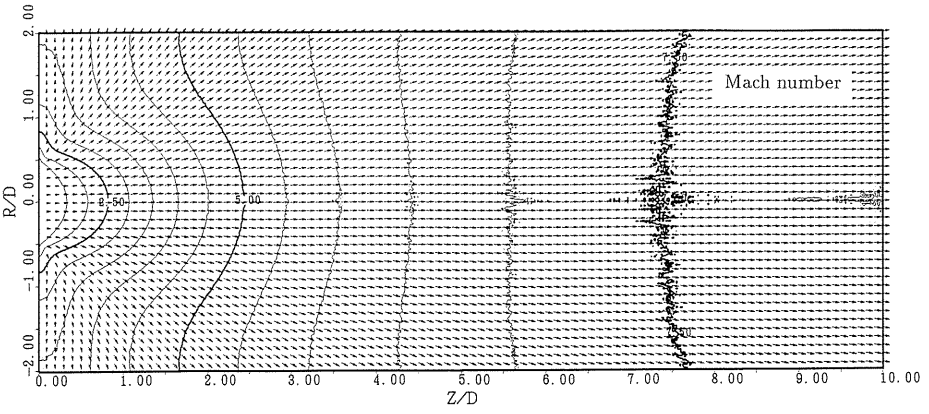

Fig. 6. Velocity vectors and Mach number contour; $Kn=0.02$.

Figs. 7 and 8 present the axial temperature T_z and the radial temperature T_r, respectively. The increment of the contours is 0.05. The minimum temperature shown in Fig. 7 is $0.2T^*$ and this fact suggests that the freezing of the temperature, T_z is beginning. On the other hand, in Fig. 8 it is $0.05T^*$ and the temperature, T_r is still decreasing. The temperature (figure is not presented here) T_θ shows a monotonic decrease and each contour is touching the contour of T_r on the axis. Since, for $z/D \geq 5$, $T_z \approx$ const, contour of temperature $T=(T_z+T_r+T_\theta)/3$ exhibits the similar behavior as T_z; that is, $T(z, r) \geq T(z, 0)$. Although his analysis is valid only in the core where the isentropic source flow is the 0th order solution, Grundy found this behavior of temperature in his analysis. Present simulation has assured that his prediction takes place in the axisymmetric expansion flow from a sonic orifice.

Properties of expansion flow along the axis of symmetry are shown in Figs. 9 to 11. Density decreases as $1/z^2$ for $z/D>1$ (Fig. 9). Fig. 10 shows that velocity is approaching about 1.96, which is less than 2 expected from the continuum flow theory. This fact is related to the

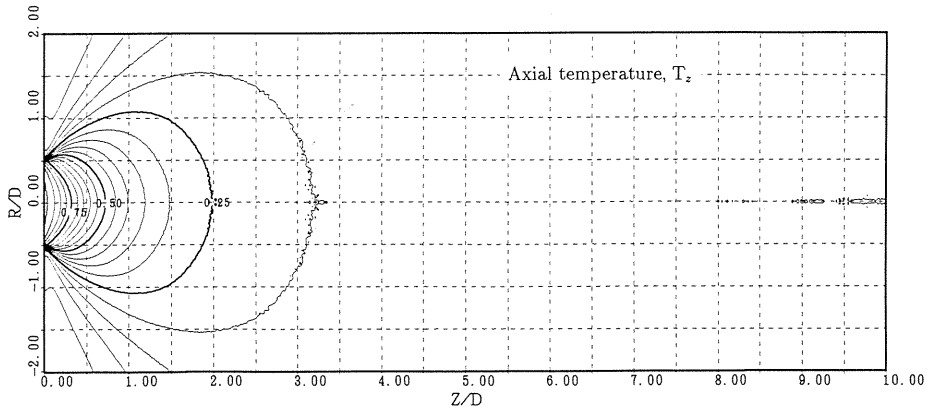

Fig. 7. Contour of radial temperature T_r; $Kn=0.02$.

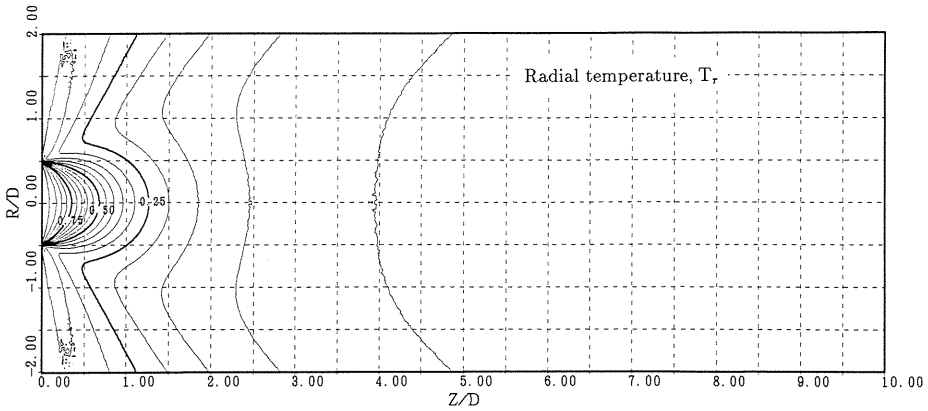

Fig. 8. Contour of axial temperature T_z; $Kn=0.02$.

abovementioned temperature freezing: Internal energy is not consumed completely to accelerate the gas. Temperature and it components T_z and $T_p=(T_r+T_\theta)/2$ are shown in Fig. 11, where $T_r=T_\theta$ on the axis of symmetry. The axial temperature seems to level off to a value between 0.16 and 0.14. Previous study on the spherical source flow[7] yields 0.16 for $\mathrm{Kn}=0.02$ where the source Knudsen number in Fig. 15 in Ref. 7 is give by $\mathrm{Kn}_D=0.65\,\mathrm{Kn}$. Fig. 11 shows that $T_z \geq T \geq T_{equil} \geq T_p$. These behaviors of the temperature and its components were also found in the previous study on the spherical source flow. Obtained values of terminal Mach number $M_{z\infty}$ on the symmetric axis showed a good agreement with the prediction of the previous study[6),7)].

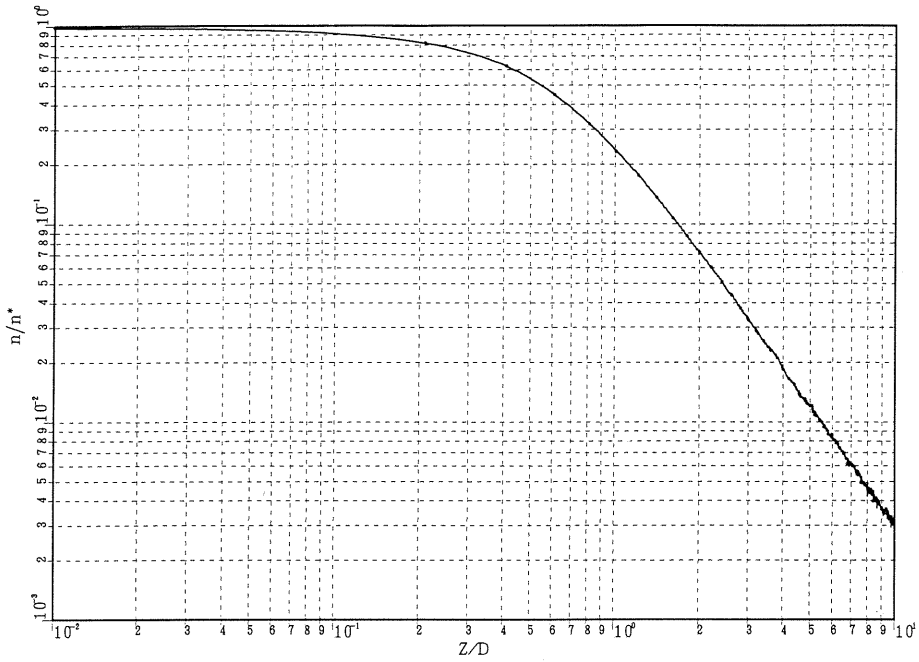

Fig. 9. Distribution of number density along the axis of symmetry; $Kn = 0.02$.

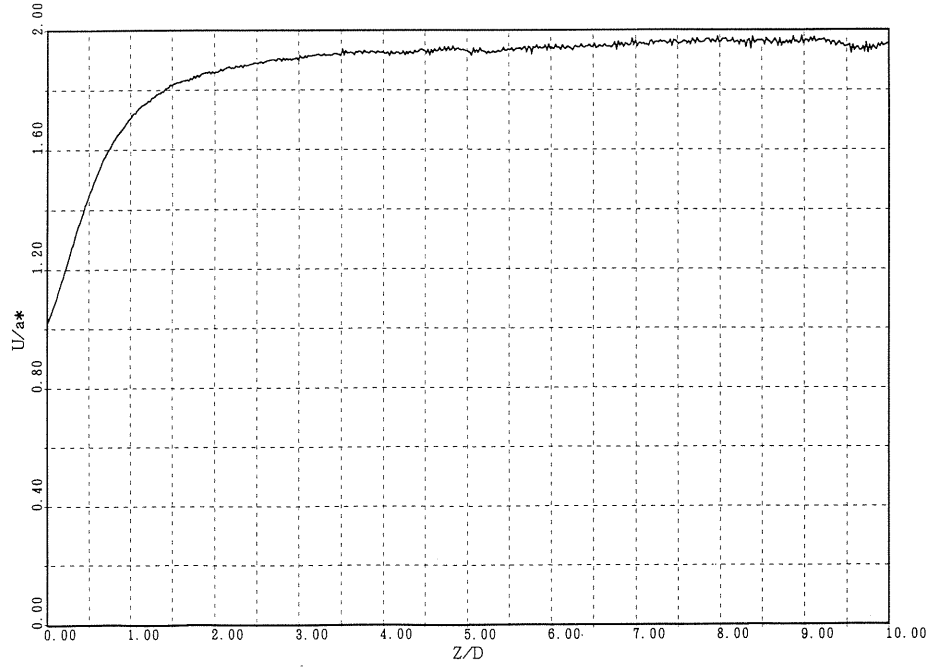

Fig. 10. Distribution of velocity along the axis of symmetry; $Kn = 0.02$.

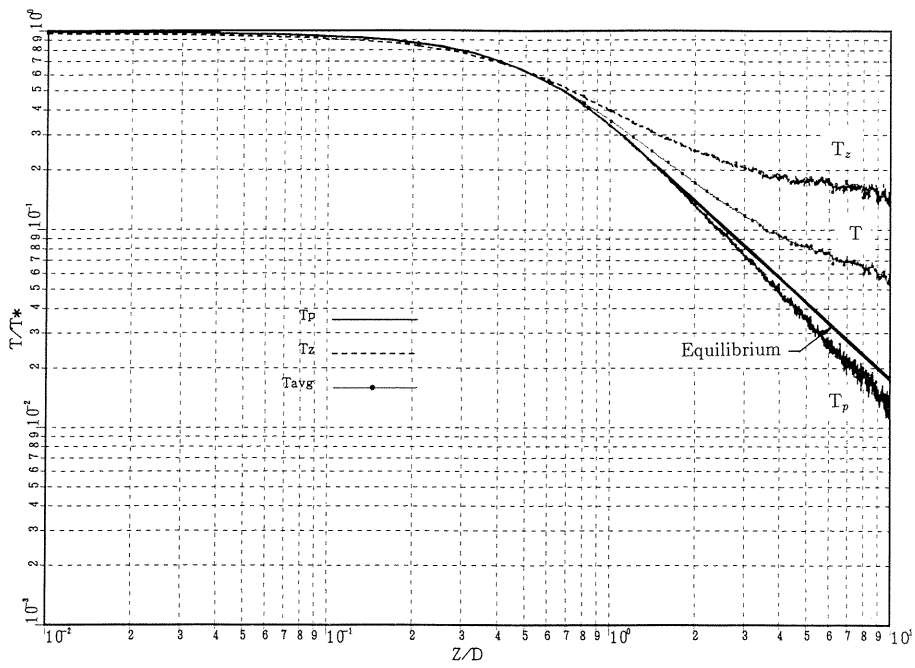

Fig. 11. Distributions of temperatures, T, T_z, and T_p along the axis of symmetry; $Kn = 0.02$.

4. Conclusions

Axisymmetric expansion flow from a circular orifice into a vacuum was studied based upon the DSMC method. The numerical simulation was carried out for the gas composed of the hard sphere molecules. It is found that the radial temperature is slightly higher than the axial temperature in the vicinity of the orifice. The degree of such a nonequilibrium decreased in accordance with the decrease of the Knudsen number Kn. For the case of Kn = 0.02 the difference between two temperatures was less than 2%. Present simulation revealed that in the vicinity of the axis of symmetry orifice flow expands like a spherical source flow but the off axis flow exhibites the peculiar features of axisymmetric expansion flow predicted by Grundy. The simulated expansion flow along the axis of symmetry includes continuum to free molecular flows. Present results, the terminal velocity, the terminal temperature, and the terminal Mach number, showed a good agreement with the previous results of spherical source flow expansion.

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