

MONTE CARLO CALCULATION OF  
RAREFIED HYPERSONIC GAS FLOW  
PAST A CIRCULAR DISC

by

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Submitted to the Department of Aeronautics and Astronautics  
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ABSTRACT

A computational study was carried out on the rarefied hypersonic gas flow past a circular disc by the use of the direct simulation Monte Carlo method for the case of Knudsen number unity and the temperature ratio between the disc and the undisturbed gas unity.

The results showed that the disturbed region was confined to a small region due to the low temperature of the wall, although the temperature disturbance extended more widely than the velocity or density disturbance. The study of the near axis flow properties clearly showed the existence of the bow shock. Both of the heat transfer rate and the pressure drag data showed small values compared with the free molecule values.

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## LIST OF SYMBOLS

$b$	miss distance impact parameter in a binary collision
$c_p$	specific heat at constant pressure
$c_v$	specific heat at constant volume
$c_m'$	most probable thermal speed, $c_m' = 1/\beta$
$\underline{c}_0$	stream velocity
$\underline{c}_m$	center of mass velocity of collision pair
$\underline{c}_r$	relative velocity between two molecules
$\underline{dc}$	volume element in velocity space, $\underline{dc} = dudvdw$
$d$	effective molecular diameter
$\underline{e}$	unit vector
$f$	normalized velocity distribution function in velocity space
$f_0$	Maxwellian velocity distribution function
$\underline{F}$	external force per unit mass
$F$	velocity distribution function in phase space
$H$	enthalpy
$k$	Boltzmann constant
$K_n$	Knudsen number
$m$	mass of a single molecule
$m_r$	reduced mass
$n$	number of density
$N$	number flux; number of molecules

$N_c$	number of collisions
$p$	pressure; normal momentum flux per unit area
$\underline{q}$	heat flux vector
$Q$	physical quantity associated with a molecule
$r$	radius; radial coordinate
$\underline{r}$	position vector
$d\underline{r}$	volume element in physical space
$R$	gas constant
$R_f$	random fraction
$s$	molecular speed ratio
$t$	time
$T$	thermodynamic temperature
$u$	velocity component in the x direction
$v$	velocity component in the r (or y) direction
$V$	volume in physical space
$w$	velocity component in the $\theta$ (or z) direction
$W_f$	weighting factor
$x$	cylindrical coordinate axis in physical space
$\beta$	reciprocal of most probable speed in an equilibrium gas
$\gamma$	ratio of specific heat
$\Delta[Q]$	collision integral
$\epsilon$	azimuth angle impact parameter in binary collision
$\eta$	exponent of inverse power law molecular force
$\theta$	angular coordinate
$\lambda$	mean free path

$\lambda_0$	mean free path in an equilibrium gas
$\nu$	collision frequency
$\nu_0$	collision frequency in an equilibrium gas
$\sigma d\Omega$	differential collision cross-section
$\sigma_T$	total collision cross-section
$\tau$	shear stress

### Superscripts and Subscripts

*	postcollision value
<sup>1, 2</sup>	particular molecules or molecular classes
fm	free molecule value
i	incident; inward
r	reflected; relative; component in the r direction
$\infty$	free stream value
w	value at wall surface
x	component in the x direction
$\theta$	component in the $\theta$ direction
0	stagnation condition



## CHAPTER 1

### INTRODUCTION

The direct simulation Monte Carlo method has proved to be a valuable tool in the study of rarefied gas flow problems [1-7]. The present paper treats the axisymmetric flow past a circular disc in the transition regime.

In the study of rarefied hypersonic transition flow over axisymmetric blunt bodies, interest has generally focused on bodies such as cylinders, hemispheres, spheres, and blunted cones, and those problems have been treated extensively from both continuum and kinetic theory viewpoints. Relatively little attention has been given, however, to flat-faced bodies, which might be regarded as the limit of maximum bluntness. Potter and Miller [8] and Bailey and Sims [9] conducted experiments to measure the characteristics of this shape in the transition regime.

Victoria and Widhopf [10] have compared the results of their finite difference solutions to the complete Navier-Stokes equations with the direct Monte Carlo calculations of hypersonic flow over a sphere with cold wall at low Reynolds numbers in order to assess the validity of the continuum approach. They found that the structure of the flow field near the body was comparable for the two calculations, but

that there were substantial differences within the outer portion of the shock wave. The stream line solution of Levinsky and Yoshihara [11], who assumed that the total disturbance region is thin compared to the radius of the body, neither velocity slip or temperature jump being considered, differs substantially from both the Monte Carlo results and the Navier-Stokes solutions over almost all the flow. This is also shown by Jain and Adimurthy [12], who examined the effects of slip boundary conditions on the thin layer and the complete Navier-Stokes solutions on the stagnation line at low Reynolds numbers.

In the present paper, direct simulation Monte Carlo results for the axisymmetric rarefied hypersonic flow past a flat-faced circular disc at Knudsen number unity are presented. Near-axis of symmetry flow properties, average heat transfer to the disc surface and pressure drag are also presented together with the density and temperature distributions in the flow field upstream of the disc.

## CHAPTER 2

### THE BOLTZMANN EQUATION AND THE MONTE CARLO METHOD

#### 2.1 The Boltzmann Equation

The Boltzmann equation can be written in the form [13]

$$\begin{aligned} \frac{\partial(nf)}{\partial t} + \underline{c} \cdot \frac{\partial(nf)}{\partial \underline{r}} + \underline{F} \cdot \frac{\partial(nf)}{\partial \underline{c}} \\ = \int_{-\infty}^{\infty} \int_0^{4\pi} n^2 (f^* f_1^* - f f_1) c_r \sigma d\Omega d\underline{c}_1 \end{aligned} \quad (2.1)$$

or

$$\begin{aligned} \frac{\partial F}{\partial t} + \underline{c} \cdot \frac{\partial F}{\partial \underline{r}} + \underline{F} \cdot \frac{\partial F}{\partial \underline{c}} \\ = \int_{-\infty}^{\infty} \int_0^{b_{\max}} \int_0^{2\pi} (F^* F_1^* - F F_1) c_r b d\epsilon d b d\underline{c}_1 \end{aligned} \quad (2.2)$$

where  $f = f(\underline{c})$  and  $F = F(\underline{c}, \underline{r}, t) = nf$ . A bar under a quantity denotes the vector quantity. The term on the right-hand side of the Boltzmann equation is called the collision term. Its integral form contrasts with the partial differential form of the terms on the left-hand side which express the space and time dependence of  $nf$ , and is responsible for much of the mathematical difficulty associated with the Boltzmann equation. On the other hand,  $nf$  is the only dependent variable

in the equation. This might be considered an advantage when comparing the Boltzmann equation with the Navier-Stokes equations of continuum gas dynamics, since these have the velocity components and two thermodynamic properties as dependent variables. However, the advantage is far outweighed by the addition of the velocity-space coordinates to the list of independent variables.

## 2.2 The Moment Method

This approach employs the moment equations which are obtained by first multiplying the Boltzmann equation by a molecular quantity, and then integrating it over velocity space. The moment equation for  $Q$  is given in the form

$$\frac{\partial}{\partial t}(n\bar{Q}) + \nabla \cdot (n\bar{cQ}) - n\underline{F} \cdot \frac{\partial \bar{Q}}{\partial \underline{c}} = \Delta[Q] \quad (2.3)$$

where

$$\Delta[Q] = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_0^{4\pi} n^2 Q (f^* f_1^* - f f_1) c_r \sigma d\Omega d\underline{c}_1 d\underline{c}. \quad (2.4)$$

A bar over a quantity denotes the average over all the velocity classes. The macroscopic quantities are defined in terms of the average of the microscopic molecular quantities  $Q$ . The substitution of various values of  $Q$  into Eq. (2.3) leads to a series of equations in the macroscopic quantities. However, the presence of  $\bar{cQ}$  in the second term means that, as  $Q$  progresses to successively higher order of  $\underline{c}$  each

equation involves a moment of still higher order. This can only be overcome by using some method of truncation, to form a determinate set of equations.

The Chapman-Enskog solution [14] of the Boltzmann equation is based on a series expansion of the distribution function  $f$  as

$$f = f_0 \left\{ 1 + a_1(K_n) + a_2(K_n)^2 + \dots \right\} \quad (2.5)$$

where the coefficients  $a_n$  are functions of  $\rho$ ,  $\underline{c}_0$ , and  $T$  only. The first-order solution is the local equilibrium of Maxwellian distribution function  $f_0$ . The conservation equations obtained by setting  $Q$  equal to  $m$ ,  $m\underline{c}$  and  $\frac{1}{2} mc^2$  are the five moment equations and reduce to the Euler equations of inviscid flow. The second-order Chapman-Enskog solution leads to the distribution function which enables the conservation equations be reduced to the Navier-Stokes equations of continuum flow. From the kinetic theory point of view, both the Euler and Navier-Stokes equations may be regarded as "five moment" solutions of the Boltzmann equation, the former being valid for the  $K_n \rightarrow 0$  limit and the latter for  $K_n \ll 1$ . If a higher order of perturbation is used, the Burnett [15,16] thirteen moment equations result. Grad [17] expanded the distribution function in Hermite polynomials, the termination scheme being to equate the higher order coefficients to zero, and obtained a different set of thirteen moment equations.

However, for the region such as boundary layers or

shock layers where the velocity, density, and temperature profiles tend to be very steep, the solutions of the inviscid fluid equations cannot be improved to describe such layers even by taking into account higher order corrections obtained by expansion in powers of a single parameter. The solutions on either side of shock layers, for example, cannot be obtained from a single set of equations which is uniformly valid both upstream and downstream flow field [18].

### 2.3 The Test Particle Monte Carlo Method

The Monte Carlo method was developed through reference to the physics of the gas flow. This is in contrast with most numerical methods which are developed through reference to the mathematical description of the flow.

The Monte Carlo method, associated primarily with Haviland [19,20] being best termed the test particle Monte Carlo method, is based on the principle that, in a steady flow maintained over a time period  $t$  for which  $t \rightarrow \infty$ , the average time spent in any region in phase space is proportional to the density distribution function  $F(x, \underline{u})$ . Thus, if the motion of a molecule can be represented analytically, and if a suitable model can be set up to represent random collisions with other molecules, the density distribution can be computed from the time spent in each element of phase space, together with any of its moments.

This can only be done if there is already a

representation of the complete flow field. Since this cannot be done directly, an iterative procedure is employed, in which the distribution obtained in the previous iteration is used as the distribution function of the "target" molecules. Following Haviland's notation applied to the one-dimensional stationary flow with no external force fields, it is equivalent to solving the Boltzman equation by the iterative scheme

$$U_x \frac{\partial}{\partial x} F^{(r)}(x, \underline{c}) = \int_{-\infty}^{\infty} d\underline{c}_1 \int_0^{b_{\max}} b db \int_0^{2\pi} d \in c_r$$

$$\cdot \left\{ F^{(r)}(x, \underline{c}^*) F^{(r-1)}(x, \underline{c}_1^*) - F^{(r)}(x, \underline{c}) F^{(r-1)}(x, \underline{c}_1) \right\}$$

(2.6)

where  $F^{(r)}$  and  $F^{(r-1)}$  are the results of successive iterations. The distribution function so chosen is stored at a discrete number of points in phase space. A large number of test molecule trajectories are computed with the assumed distribution for the computation of typical intermolecular collisions. When convergence has been obtained, so that  $F^{(r)} = F^{(r-1)} = F$ , we have a solution to the Boltzmann equation:

$$U_x \frac{\partial}{\partial x} F(x, \underline{c}) = \int_{-\infty}^{\infty} d\underline{c}_1 \int_0^{b_{\max}} b db \int_0^{2\pi} d \in c_r$$

$$\cdot \left\{ F(x, \underline{c}^*) F(x, \underline{c}_1^*) - F(x, \underline{c}) F(x, \underline{c}_1) \right\}.$$

(2.7)

## 2.4 The Direct Simulation Monte Carlo Method

The alternative to the test particle approach is to follow the trajectories of a very large number of simulated molecules simultaneously. This process commences from a specified initial state and then proceeds through a physically real unsteady process. An initial estimate of the flow field is not required and there is no iterative process.

This direct simulation scheme was first adopted by Alder and Wainwright [21] treating the molecular dynamics as completely deterministic. Each time a single molecule is considered, all other molecules must be examined as possible collision partners. This process requires computing time proportional to the square of the total number of molecules in the region and all but the most elementary problems are beyond the scope of the method.

Bird [22] first applied the direct simulation Monte Carlo method to the homogeneous gas relaxation problem, adopting probabilistic rather than deterministic procedures for the computation of collisions, thus making the computing requirement manageable.

This direct simulation Monte Carlo method by Bird is adopted in the present paper to calculate the transition regime gas flow past a circular disc and is discussed in detail in the following chapters.



## CHAPTER 3

### FUNDAMENTAL RELATIONS

In this chapter, some fundamental relations of the kinetic theory will be reviewed so that they can be referred to and be used directly in the following chapters.

#### 3.1 The Molecular Model

For sufficiently low densities, the molecular spacing is large compared with the effective molecular diameter. Under these circumstances, only a small portion of space is occupied by molecules. Each molecule moves, for the most part, freely in space outside the range of influence of other molecules. Moreover, when it suffers a collision, it is overwhelmingly likely to be a binary collision involving only one other molecule. This situation defines a dilute gas.

The time scale of the microscopic process is set by the mean collision time which is, by definition, the mean time interval between the successive collisions suffered by a typical molecule. The reciprocal of this quantity is called the mean collision rate or collision frequency per molecule. The mean collision rate is obtained by summing the number of collisions for a test molecule per unit time with a class  $c$  molecule over all velocity classes and therefore over all

values of relative velocity. That is,

$$v = n\overline{\sigma_T c_r} \quad (3.1)$$

where  $n$  is number density,  $\sigma_T$  is total collision cross-section and  $c_r$  is relative speed. A bar over a quantity denotes the average value over all molecules in the sample gas.

The total number of collisions per unit time per unit volume of gas is given by

$$N_c = \frac{1}{2} nv = \frac{1}{2} n^2 \overline{\sigma_T c_r}. \quad (3.2)$$

The symmetry factor  $1/2$  is introduced because each collision involves two molecules. The mean free path is the average distance traveled by a molecule between successive collisions and is therefore equal to the mean speed  $\overline{c^T}$  of a molecule divided by the mean collision rate, i.e.,

$$\lambda = \overline{c^T}/v = \{n(\overline{\sigma_T c_r}/\overline{c^T})\}^{-1}. \quad (3.3)$$

If  $\sigma_T$  is regarded as a constant, the mean collision rate and the mean free path are

$$v = n\overline{\sigma_T c_r} = n\pi d^2 \overline{c_r} \quad (3.4)$$

and

$$\lambda = \{(\overline{c_r}/\overline{c^T})\pi d^2 n\}^{-1}. \quad (3.5)$$

The mean free path is defined in a frame of reference moving with the free stream velocity of the gas. The prime on the mean molecular speed  $\bar{c}'$  denotes that this quantity is measured relative to the stream velocity.

### 3.2 Binary Collision

The precollision velocities of the two collision partners in a typical binary elastic collision may be denoted as  $\underline{c}_1$  and  $\underline{c}_2$ . The postcollision velocities  $\underline{c}_1^*$  and  $\underline{c}_2^*$  will be determined. Using the relationship of conservation of linear momentum and energy in the collision, we get

$$m_1 \underline{c}_1 + m_2 \underline{c}_2 = m_1 \underline{c}_1^* + m_2 \underline{c}_2^* = (m_1 + m_2) \underline{c}_m \quad (3.6)$$

and

$$m_1 c_1^2 + m_2 c_2^2 = m_1 c_1^{*2} + m_2 c_2^{*2} \quad (3.7)$$

where  $m_1$  and  $m_2$  denote the masses of the two molecules and  $\underline{c}_m$  is the velocity of the center of mass of the pair of molecules. The precollision and postcollision relative velocities between the molecules are given by

$$\underline{c}_r = \underline{c}_1 - \underline{c}_2$$

and

$$\underline{c}_r^* = \underline{c}_1^* - \underline{c}_2^*$$

} (3.8)

Eqs. (3.6) and (3.8) may be combined to give

$$\left. \begin{aligned} \underline{c}_1 &= \underline{c}_m + m_2 \underline{c}_r / (m_1 + m_2) \\ \underline{c}_2 &= \underline{c}_m - m_1 \underline{c}_r / (m_1 + m_2). \end{aligned} \right\} (3.9)$$

As can be noticed from Eq. (3.9), the collision is planar in the center of mass frame. Similarly, postcollision velocities may be obtained from Eqs. (3.6) and (3.8) as

$$\left. \begin{aligned} \underline{c}_1^* &= \underline{c}_m + \frac{m_2}{m_1 + m_2} \underline{c}_r^* \\ \underline{c}_2^* &= \underline{c}_m - \frac{m_1}{m_1 + m_2} \underline{c}_r^*. \end{aligned} \right\} (3.10)$$

This shows that the postcollision velocities are also parallel in the center of mass frame. The conservation of angular momentum requires that the projected distance between postcollision velocities be equal to the projected distance between the precollision velocities.

Eqs. (3.9) and (3.10) show that

$$\left. \begin{aligned} m_1 c_1^2 + m_2 c_2^2 &= (m_1 + m_2) c_m^2 + m_r c_r^2 \\ \text{and} \\ m_1 c_1^{*2} + m_2 c_2^{*2} &= (m_1 + m_2) c_m^2 + m_r c_r^{*2} \end{aligned} \right\} (3.11)$$

where

$$m_r = \frac{m_1 m_2}{m_1 + m_2} \quad (3.12)$$

is called the reduced mass. A comparison of Eq. (3.11) with

the energy equation (3.7) shows that the magnitude of the relative velocity is unchanged by the collision, i.e.,

$$c_r^* = c_r. \quad (3.13)$$

Since both  $\underline{c}_m$  and  $\underline{c}_r$  may be calculated from the precollision velocities, the determination of postcollision velocities reduces to the calculation of the change in direction of the relative velocity vector.

### 3.3 Distribution Function in an Equilibrium Gas

The equilibrium velocity distribution function is defined as

$$f_0 = \frac{\beta^3}{\pi^{3/2}} \exp(-\beta^2 c'^2) \quad (3.14)$$

where

$$\beta = (2RT)^{-1/2} = \{m/(2kT)\}^{1/2}. \quad (3.15)$$

The fraction of molecules that are located within a velocity space element of volume  $d\underline{c}$  and located at  $\underline{c}'$ , therefore, is

$$\frac{dn}{n} = \frac{\beta^3}{\pi^{3/2}} \exp(-\beta^2 c'^2) d\underline{c}'. \quad (3.16)$$

The equilibrium speed distribution function is defined as

$$f_{c'} = \frac{4\beta^3 c'^2}{\pi^{3/2}} \exp(-\beta^2 c'^2) \quad (3.17)$$

The function  $f_{c'}$  is zero when  $c'$  is zero, increases to a maximum value when  $\beta c'$  is unity, and then decreases as  $c'$  increases. The parameter  $\beta$  is, therefore, the reciprocal of the most probable molecular thermal speed  $c'_m$ , i.e.,

$$c'_m = 1/\beta. \quad (3.18)$$

The average of any quantity depending upon the molecular thermal speed may be obtained through the mean value principle. The average thermal speed  $\bar{c}'$  is

$$\bar{c}' = \int_0^{\infty} c' f_{c'} dc' = \frac{4}{\pi^{1/2}} \beta^3 \int_0^{\infty} c'^3 \exp(-\beta^2 c'^2) dc'$$

or

$$\bar{c}' = \frac{2}{\pi^{1/2} \beta}. \quad (3.19)$$

The fraction of molecules with a velocity component within a given range, irrespective of the magnitude of other components, is obtained by integrating Eq. (3.14) over these other velocity components. The fraction of molecules with a thermal velocity component in the x direction between  $u'$  and  $u' + du'$  is

$$\begin{aligned} & \frac{\beta^3}{\pi^{3/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\{-\beta^2 (u'^2 + v'^2 + w'^2)\} dv' dw' du' \\ & = \frac{\beta}{\pi^{1/2}} \exp(-\beta^2 u'^2) du'. \end{aligned} \quad (3.20)$$

The distribution function for a thermal velocity component is, therefore,

$$f_{u'} = \frac{\beta}{\pi^{1/2}} \exp(-\beta^2 u'^2). \quad (3.21)$$

### 3.4 Collisional Quantities in an Equilibrium Gas

General expressions for the mean collision rate and mean free path in a dilute gas obtained in the previous section involve the mean value of the product of the collision cross-section and the relative speed. For the special case of hard sphere molecule with a fixed cross-section, the mean value of the magnitude of relative velocity is the only one that has to be taken into consideration.

The relative velocity in a binary collision is  $\underline{c}_R = \underline{c}_1 - \underline{c}_2$ , where the subscript 1 and 2 denote the two molecules that are involved in a collision. Assuming molecular chaos, the two particle distribution function is equal to the product of the two single-particle distribution functions  $f_1$  and  $f_2$ . The required mean value is then

$$\overline{c}_R = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} c_R f_1 f_2 d\underline{c}_1 d\underline{c}_2 \quad (3.22)$$

and for an equilibrium gas

$$\overline{c}_R = \frac{m_1 m_2}{(2\pi kT)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} c_R \exp\left\{-\frac{(m_1 c_1^2 + m_2 c_2^2)}{2kT}\right\} d\underline{c}_1 d\underline{c}_2. \quad (3.23)$$

This equation can be integrated to give

$$\overline{c_r} = \frac{2}{\pi^{1/2}} \left( \frac{2kT}{m_r} \right)^{1/2}. \quad (3.24)$$

For a simple gas,  $m_r = m/2$  and the result is

$$\overline{c_r} = 2^{3/2} / (\pi^{1/2} \beta) = 2^{1/2} \overline{c^r}. \quad (3.25)$$

The mean collision rate per molecule in an equilibrium simple gas of hard sphere molecules is then given by the substitution of Eq. (3.25) into Eq. (3.4), i.e.,

$$v_0 = 2^{1/2} \pi d^2 n \overline{c^r}. \quad (3.26)$$

The number of collisions per unit time and unit volume follows from Eqs. (3.2) as

$$N_{c_0} = 2^{-1/2} \pi d^2 n^2 \overline{c^r}. \quad (3.27)$$

The mean free path in an equilibrium gas of hard sphere molecules is then given by Eqs. (3.26) and (3.3) as

$$\lambda_0 = (2^{1/2} \pi d^2 n)^{-1}. \quad (3.28)$$

### 3.5 Flux Quantities in an Equilibrium Gas

The flux of molecular quantities across a surface element in an equilibrium gas will be considered. The stream velocity is inclined at the angle  $\theta$  to the unit normal vector  $\underline{e}$  to the surface element, as shown in Figure 3.1.



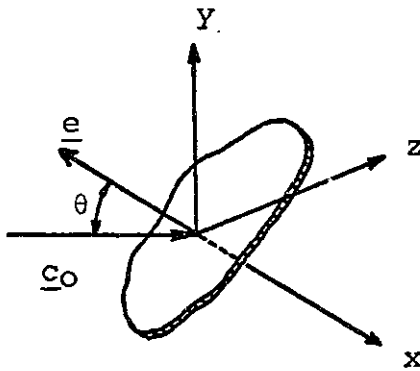


Fig. 3.1.--Molecular flux across a surface element.

Without loss of generality, we may choose Cartesian coordinates such that the stream velocity lies in the  $x,y$ -plane and the surface element lies in the  $y,z$ -plane, with the  $x$  axis in the negative  $\underline{e}$  direction. Each molecule has velocity components

$$\left. \begin{aligned} u &= u' + c_0 \cos\theta \\ v &= v' + c_0 \sin\theta \end{aligned} \right\} (3.29)$$

and

$$w = w'.$$

Therefore, the inward (i.e., in the negative  $\underline{e}$  direction) flux of some quantity  $Q$  is

or

$$\left. \begin{aligned} n\bar{Q}u \\ n \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_0^{\infty} Q u f d u d v d w \end{aligned} \right\} (3.30)$$

where consideration has been limited to those molecules moving in the negative  $\underline{e}$  direction. For an equilibrium gas, the function  $f_0$  may be substituted from Eq. (3.14) to give the inward flux of the quantity  $Q$  across the element as

$$\frac{n\beta^3}{\pi^{3/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_0^{\infty} Qu \exp\{-\beta^2(u'^2 + v'^2 + w'^2)\} du'dv'dw' \quad (3.31)$$

per unit area per unit time. Eq. (3.29) enables this to be written in terms of the stream velocity and the thermal velocity components only, i.e.,

$$\begin{aligned} \frac{n\beta^3}{\pi^{3/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-c_0 \cos \theta}^{\infty} & \cdot Q(u' + c_0 \cos \theta) \\ & \cdot \exp\{-\beta^2(u'^2 + v'^2 + w'^2)\} du'dv'dw'. \end{aligned} \quad (3.32)$$

The inward number flux  $N_i$  to the element is obtained by setting  $Q = 1$  in Eq. (3.32). The variables in the multiple integral may be separated to give

$$\begin{aligned} N_i = \frac{n\beta^3}{\pi^{3/2}} \int_{-\infty}^{\infty} \exp(-\beta^2 w'^2) dw' \int_{-\infty}^{\infty} \exp(-\beta^2 v'^2) dv' \\ \cdot \int_{-c_0 \cos \theta}^{\infty} (u' + c_0 \cos \theta) \exp(-\beta^2 u'^2) du'. \end{aligned} \quad (3.33)$$

The right-hand side of this equation can be integrated to give

$$N_i = \frac{n}{2\beta\pi^{1/2}} [\exp(-s^2 \cos^2 \theta) + \pi^{1/2} s \cos \theta \{1 + \operatorname{erf}(s \cos \theta)\}] \quad (3.34)$$

where

$$s = c_0 \beta = c_0 / c_m' = c_0 / (2RT)^{1/2}$$

is called the molecular speed ratio. For a stationary gas where  $c_0 = s = 0$ , this reduces to

$$N_i = \frac{n}{2\beta\pi^{1/2}} = \frac{1}{4} n\bar{c}. \quad (3.35)$$

The inward normal momentum flux  $p_i$  to the element is obtained by setting  $Q = mu = m(u' + c_0 \cos\theta)$  in Eq. (3.32) as

$$p_i = \frac{mn\beta^3}{\pi^{3/2}} \int_{-\infty}^{\infty} \exp(-\beta^2 w'^2) dw' \int_{-\infty}^{\infty} \exp(-\beta^2 v'^2) dv' \\ \cdot \int_{-c_0 \cos\theta}^{\infty} (u' + c_0 \cos\theta)^2 \exp(-\beta^2 u'^2) du'$$

or

$$p_i = \frac{\rho}{2\pi^{1/2}\beta^2} \left[ s \cos\theta \exp(-s^2 \cos^2\theta) \right. \\ \left. + \pi^{1/2} \{1 + \operatorname{erf}(s \cos\theta)\} \left[ \frac{1}{2} + s^2 \cos^2\theta \right] \right]. \quad (3.36)$$

The inward parallel momentum flux  $\tau_i$  to the element is obtained by setting  $Q = mv = m(v' + c_0 \sin\theta)$  in Eq. (3.32) as

$$\tau_i = \frac{mn\beta^3}{\pi^{3/2}} \int_{-\infty}^{\infty} \exp(-\beta^2 w'^2) dw' \int_{-\infty}^{\infty} (v' + c_0 \sin\theta) \exp(-\beta^2 v'^2) dv' \\ \cdot \int_{-c_0 \cos\theta}^{\infty} (u' + c_0 \cos\theta) \exp(-\beta^2 u'^2) du'$$

or

$$\tau_i = \frac{\rho}{2\pi^{3/2}\beta^2} s \sin\theta [\exp(-s^2 \cos^2\theta) + \pi^{1/2} s \cos\theta \{1 + \operatorname{erf}(s \cos\theta)\}]. \quad (3.37)$$

The inward translational energy flux  $q_i$  to the element can be obtained by setting  $Q = \frac{1}{2} mc^2 = \frac{1}{2} m(u^2 + v^2 + w^2)$  in Eq. (3.32) as

$$q_i = \frac{mn\beta^3}{2\pi^{3/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-c_0 \cos\theta}^{\infty} \{(u' + c_0 \cos\theta)^2 \\ + (v' + c_0 \sin\theta)^2 + w'^2\} \\ \cdot (u' + c_0 \cos\theta) \exp\{-\beta^2(u'^2 + v'^2 + w'^2)\} du' dv' dw'$$

or

$$q_i = \frac{\rho}{4\pi^{3/2}\beta^3} \left[ (s^2 + 2) \exp(-s^2 \cos^2\theta) \right. \\ \left. + \pi^{1/2} s \cos\theta \left( s^2 + \frac{5}{2} \right) \{1 + \operatorname{erf}(s \cos\theta)\} \right]. \quad (3.38)$$

From the same discussion that leads to Eqs. (3.30), (3.31), and (3.32), the fraction of molecules with velocity

normal to the element between  $u'$  and  $u' + du'$ , irrespective of the magnitude of the other components, is obtained as

$$\frac{dn}{n} = \frac{\beta^3}{\pi^{3/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (u' + c_0 \cos \theta) \cdot \exp\{-\beta^2(u'^2 + v'^2 + w'^2)\} du' dv' dw' \quad (3.39)$$

or

$$\frac{dn}{n} = \frac{\beta}{\pi^{1/2}} (u'_n + c_0 \cos \theta) \exp(-\beta^2 u'_n{}^2) du'_n. \quad (3.40)$$

Here  $u'$  has been replaced by  $u'_n$  in order to make it clear that this is the normal component. The distribution function for the thermal velocity component  $u'_n$  normal to the boundary element is, therefore,

$$f_{u'_n} = \frac{\beta}{\pi^{1/2}} (u'_n + c_0 \cos \theta) \exp(-\beta^2 u'_n{}^2) \quad (3.41)$$

or

$$f_{\beta u'_n} = \frac{1}{\beta \pi^{1/2}} (\beta u'_n + s_n) \exp(-\beta^2 u'_n{}^2) \quad (3.42)$$

where  $s_n$  is the component of the stream velocity normal to the boundary element.

The distribution function for a reflecting velocity component normal to a diffusely reflecting surface follows from Eq. (3.30). This is

$$f_u = C \exp(-\beta^2 u^2) \quad (3.43)$$

where C is a constant. Now

$$f_u du = C \exp(-\beta^2 u^2) du = \frac{1}{2} C \exp(-\beta^2 u^2) d(u^2)$$

so that the distribution function for the square of the normal velocity component is

$$f_{u^2} = \frac{1}{2} C \exp(-\beta^2 u^2).$$

The constant C may be evaluated through the normalization condition of Eq. (A.4) to give

$$f_{\beta^2 u^2} = \exp(-\beta^2 u^2). \quad (3.44)$$

### 3.6 Free Molecule Flow Properties

Since the results from the free molecule theory provide the limit  $K_n \rightarrow \infty$ , they serve as important references and are used during the data reduction in Chapter 6. The surface properties follow from the application of the flux equation in Section 3.5 to the incident and reflected molecules. The reflected flux is discussed for the diffuse reflection. The subscripts i and r will be used to denote the incident and reflected molecular streams.

The values of the inward normal momentum flux  $p_i$ , inward parallel momentum flux  $\tau_i$ , and inward translational energy flux  $q_i$  are given directly by Eqs. (3.36), (3.37),

and (3.38), respectively.

In diffuse reflection, the molecules are brought to rest relative to the surface and are reemitted with the equilibrium distribution corresponding to a temperature  $T_r$ . The quantities  $p_r$  and  $q_r$  are, therefore, given by the flux equations for stationary gas with  $s = 0$ . The reflected parallel momentum  $\tau_r$  is, of course, zero. From Eq. (3.36)

$$p_r = \frac{n_r m}{4\beta_r^2} \quad (3.45)$$

and, from Eq. (3.38),

$$q_r = \frac{n_r m}{2\pi^{1/2}\beta_r^3}. \quad (3.46)$$

The number density  $n_r$  may be found from the condition that the net number flux to the element is zero, i.e.,

$$N_{\text{net}} = N_i + N_r = 0. \quad (3.47)$$

Substituting from Eq. (3.34) for the incident number flux and from Eq. (3.35) for the reflected number flux into Eq. (3.45), we have

$$\frac{n_\infty}{2\pi^{1/2}\beta_\infty} [\exp(-s^2 \cos^2 \theta) + \pi^{1/2} s \cos \theta \{1 + \text{erf}(s \cos \theta)\}] - \frac{n_r}{2\pi^{1/2}\beta_r} = 0.$$

Therefore,

$$n_r = n_\infty \left( \frac{T_\infty}{T_r} \right)^{\frac{1}{2}} \left[ \exp(-s^2 \cos^2 \theta) + \pi^{\frac{1}{2}} s \cos \theta \{1 + \operatorname{erf}(s \cos \theta)\} \right], (3.48)$$

The above results may be combined to give the following results for the pressure, shear stress, and heat transfer at the surface.

$$\begin{aligned} \frac{p}{p_\infty} &= \frac{2\beta_\infty^2 (p_i + p_r)}{\rho_\infty} \\ &= \left[ \frac{s \cos \theta}{\pi^{\frac{1}{2}}} + \frac{1}{2} \left( \frac{T_r}{T_\infty} \right)^{\frac{1}{2}} \right] \exp(-s^2 \cos^2 \theta) \\ &\quad + \left[ \frac{1}{2} + s^2 \cos^2 \theta + \frac{\pi^{\frac{1}{2}} s \cos \theta}{2} \left( \frac{T_r}{T_\infty} \right)^{\frac{1}{2}} \right] \{1 + \operatorname{erf}(s \cos \theta)\}, (3.49) \end{aligned}$$

$$\begin{aligned} \frac{\tau}{p_\infty} &= \frac{2\beta_\infty^2 \tau_i}{\rho_\infty} \\ &= \frac{s \sin \theta}{\pi^{\frac{1}{2}}} \left[ \exp(-s^2 \cos^2 \theta) + \pi^{\frac{1}{2}} s \cos \theta \{1 + \operatorname{erf}(s \cos \theta)\} \right], (3.50) \end{aligned}$$

and

$$\begin{aligned} \frac{\beta_\infty^3 q}{\rho_\infty} &= \frac{\rho_\infty^3 (q_i - q_r)}{\rho_\infty} \\ &= \frac{1}{4\pi^{\frac{1}{2}}} \left\{ (s^2 + 2) - 2 \left( \frac{T_r}{T_\infty} \right) \right\} \exp(-s^2 \cos^2 \theta) \\ &\quad + \left\{ \left( \frac{s^2}{4} + \frac{5}{8} \right) - \frac{1}{2} \left( \frac{T_r}{T_\infty} \right) \right\} s \cos \theta \{1 + \operatorname{erf}(s \cos \theta)\}. (3.51) \end{aligned}$$



## CHAPTER 4

### THE DIRECT SIMULATION MONTE CARLO METHOD

#### 4.1 General Procedure

The direct simulation Monte Carlo method is a technique for the computer modeling of a real gas flow. The process commences from some initial configuration and computes the trajectories of some thousands of simulated molecules. The simulated molecule is regarded as being representative of some very large number of molecules in the real gas in a particular volume element. The simulated region of physical space is divided into an array of cells, the size of which are chosen so that the gradients of any flow properties are small across the cell. Macroscopic quantities are sampled in each cell. The velocity components and position coordinates of the simulated molecules are stored in the computer and are modified with time as the molecules are followed through representative collisions and boundary interactions in the simulated physical space. The ideal procedure would be to move the molecules simultaneously with the computation of collisions. However, there is expected to be a considerable saving in computation time if the locations of the molecules remain unchanged while a number of collisions appropriate to some time interval is calculated.

Time is advanced in discrete steps of magnitude  $\Delta t_m$ , such that  $\Delta t_m$  is small compared with a mean collision time per molecule. Then, the molecular motion and collision are decoupled over the small time interval  $\Delta t_m$  by repeating the following steps:

- (a) All of the molecules are moved through distances appropriate to their velocity components and the time interval. Appropriate action is taken if the molecule crosses boundaries representing solid surfaces or the outer boundary of the flow. Appropriate action is taken when it is needed, if the molecule crosses a cell boundary. New molecules are generated at boundaries across which there is an inward flux.
- (b) A representative set of collisions, appropriate to  $\Delta t_m$ , is calculated among the molecules. The pre-collision velocity components of the molecules involved in the collisions are replaced by the post-collision values. The position coordinates of the molecules are not changed at this point due to the reason stated above. Since the gradients of the flow properties are small across each cell, any one of the molecules in a cell can be regarded as a sample of the molecules at any instant at that location. This enables the relative positions of the molecules within the cell to be disregarded when the collision pairs are chosen.

The sampling interval is chosen as some multiples of the time interval  $\Delta t_m$ . Flow chart of the procedures is shown in Figure 4.1. In the following sections, detail procedure

will be discussed with our attention confined to hard sphere molecule model.

#### 4.2 Computation of Collision

The collision probability for a particular pair of molecules is proportional to  $\sigma_T c_r$ , as can be shown by a discussion similar to that which leads to eqn (3.4). Since  $\sigma_T$  can be regarded as a constant and equated to  $\pi d^2$  for a hard sphere molecule, the collision probability is proportional to the relative speed  $c_r$  only and the representative collision must be chosen on that basis.

Appropriate number of collisions  $N_t$  over time period  $\Delta t_m$  in a cell is determined using eqns (3.1) and (3.2)

$$Nt = \frac{1}{2} N_m n \overline{\sigma_T c_r} \Delta t_m$$

or, again using eqn (3.4) for hard sphere molecules

$$Nt = (Nm/2) \pi d^2 n \overline{c_r} \Delta t_m \quad (4.1)$$

where  $N_m$  is the number of molecules in the cell. One way of dealing with the problem would be to calculate either the number  $N_t$  of collisions per  $\Delta t_m$  or sample the number from a normal distribution with  $N_t$  as a mean when appropriate. However, noticing the term  $\overline{c_r}$  in the right hand side of the equation, the computation time required to calculate the mean value  $\overline{c_r}$  is nearly proportional to the square of the number of molecules

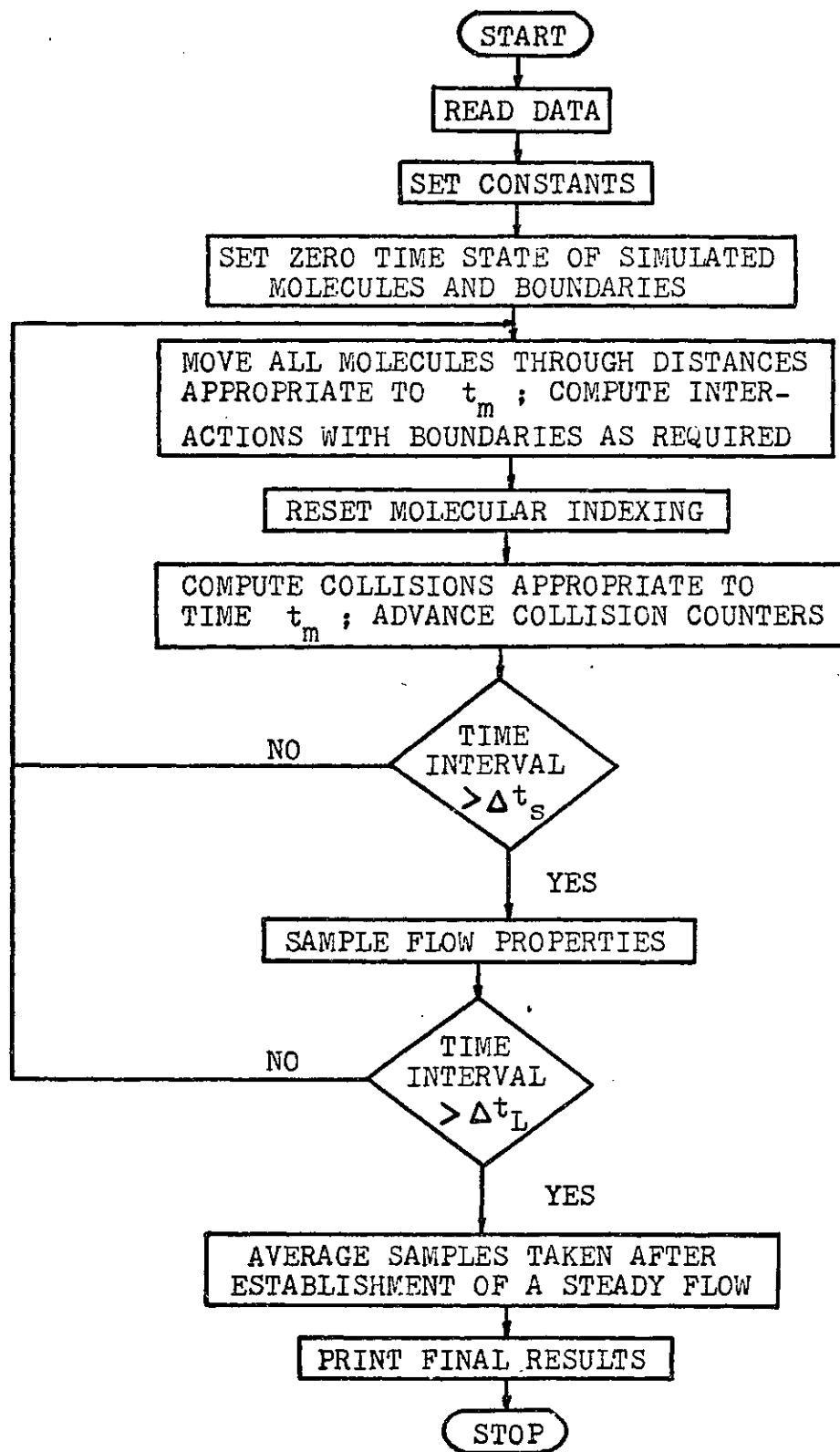


FIG. 4.1 Flow chart of the direct simulation Monte Carlo method

in the cell and is undesirable. This step can completely be avoided by advancing a time counter for each cell at each collision by

$$\Delta t_c = (2/Nm) (\pi d^2 n c_r)^{-1} \quad (4.2)$$

Formal proof that this leads to eqn (4.1) over a large number of samples is provided in [Appendix F, 23]. Since the overall time for the entire flow field is advanced by  $\Delta t_m$ , sufficient number of collisions for each cell will be calculated to keep the cell time counters concurrent with the overall flow time.

The post collision velocity components are calculated through a direct application of the result of the classical collision mechanics that all the directions are equally likely for the relative velocity  $\underline{c}_r^*$  after collision. The magnitude of this quantity is unaffected as shown in eqn (3.13) by an elastic collision. An element of solid angle in polar coordinates with  $\theta$  as the polar angle and  $\phi$  as the azimuth angle, is  $\sin\theta d\theta d\phi$ . Therefore,  $\phi$  is uniformly distributed between 0 and  $2\pi$ , while  $\theta$  is between 0 and  $2\pi$  with a distribution function  $f_\theta = \sin\theta$ . Now the fraction of angle between  $\theta$  and  $\theta+d\theta$  is

$$f_\theta d\theta = \sin\theta d\theta = -d(\cos\theta)$$

and this is also the fraction of molecules with cosines between  $\cos\theta$  and  $\cos\theta + d(\cos\theta)$ . Therefore,

$$f_{\cos\theta} d(\cos\theta) = -d(\cos\theta). \quad (4.3)$$

so that  $f_{\cos\theta}$  is a constant and  $\cos\theta$  is uniformly distributed between -1 and +1.

### 4.3 Weighting Factor

In an axially symmetric flow, the volume of a cell must be calculated from the appropriate annulus. The volumes of cells located at large distances from the axis of symmetry are therefore large in comparison with those of cells of similar cross sectional area near the axis. If the density is similar in each of those cells, the number of simulated molecules and consequently the sample size for macroscopic flow properties is either excessively large away from the axis of symmetry or excessively small near the axis. This large disparities in the sample size is undesirable because a small sample leads to large degree of statistical scatter in the results, while a large sample leads to excessive computation time.

Each simulated molecule may be regarded as a representative of some large number of real molecules. There is no reason why the ratio of numbers of real to simulated molecules has to be the same in all parts of flow field. This principle allows us to use weighting factors. The weighting factors are mainly to be used to compensate for large disparities in cell volume, although they can be used also to compensate for large disparities in density distribution. In either case, the purpose of the use of weighting factors is to avoid large variations in sample size over the entire flow field.

A weighting factor is assigned to each cell. They are normalized so that the minimum value is unity. If the weighting factor for cell  $n$  is  $W_n$ , each molecule in the cell represents

$W_n$  weighted molecules. The relationship between the weighted molecules and the real molecules is stated as follows. The number  $N_M$  of simulated molecules in a flow field of  $N_C$  cells is

$$N_M = \sum_{n=1}^{N_C} (n_n V_n / W_n) \quad (4.4)$$

where  $n_n$  and  $V_n$  are the number density and the volume in cell  $n$ . When a molecule moves from a cell with weighting factor  $W_n$  to one with weighting factor  $W_m$ , provision must be made either to duplicate or remove the molecule. The number of molecules in the new cell should be equal to  $W_n / W_m$  and, since this will generally not be an integer, the removal or duplication is based on an acceptance-rejection method. The number density in an initially uniform flow containing  $N_M$  molecules is obtained from eqn (4.4) as

$$n^\infty = N_M \left\{ \sum_{n=1}^{N_C} (V_n / W_n) \right\}^{-1} \quad (4.5)$$

#### 4.4 Molecular Indexing Scheme

In general, a flow field has open boundaries and provision must be made for a systematic change in the number of simulated molecules during an unsteady process. All the molecules in the simulated space are distinguished by the molecule numbers assigned to them and are ordered in a molecular array. A molecule is considered to be lost if it moves out across the

boundary. Once the locations of the molecules are settled, the numbers (addresses in the molecular array) of the molecules in a particular cell are stored in a cross reference array, so that the properties of the molecules in the cell can easily be referenced. Reordering of all the molecules in the simulated region should be made whenever molecular properties in the cells are referred.

#### 4.5 Initial Configuration

The steady state solution is found as the large time limit of the solution of the unsteady flow that follows the instantaneous insertion of a body into a uniform stream. An alternative initial configuration would be a body in a vacuum, with the stream commencing to enter from the upstream boundary at time zero. In either case, the sampling of the required steady flow properties, therefore, will not be commenced until some time after the start of the program.

In this paper the former initial configuration is used. For each cell, some specified number of simulated molecules are set up, in thermal equilibrium, to form a uniform stream of the required speed ratio.



## CHAPTER 5

### MONTE CARLO CALCULATION OF RAREFIED HYPERSONIC GAS FLOW PAST A CIRCULAR DISC

#### 5.1 Definition of the Problem

Assuming a uniform parallel flow, a circular disc is placed normal to the flow direction as shown in Fig. 5.1. The temperature of the disc is maintained at a constant value. The disc has a diffusely reflecting surface, that is to say, every molecule striking the disc is completely accommodated when it is reflected or re-emitted from the surface. For a specific Knudsen number  $K_n$  and speed ratio  $s$ , the steady state flow properties of the flow field as well as mass, momentum and heat flux to the disc are sought in this work. The flow is always unsteady since we are on a molecular basis. However, the boundary conditions may be considered such that the steady state can be obtained as a large time limit of an unsteady process. It is assumed that whenever a molecule strikes the wall surface, it is immediately re-emitted.

#### 5.2 Simulated Region of Physical Space

The boundary conditions of this problem at infinity must be such that the distributions are Maxwellian, the flow properties being those in a translating equilibrium gas. One of the difficulties is how to replace the boundaries at infinity

by boundaries relatively close to the disc. If the boundaries are too close, it is no longer appropriate to assume a Maxwellian. And if they are too far, it requires excessive amount of computation time, because the appropriate size of each cell has to be determined such that gradients of the flow properties over a cell should not be large and, accordingly, too large a flow region requires an excessive number of cells and of simulated molecules.

An estimate for the appropriate location of the boundaries upstream and radially is made from the flow field data obtained for a sphere by Bird<sup>[1]</sup> and Vogenitz et al<sup>[2]</sup>. The boundary downstream is chosen to coincide with the plane in which the disc is located since the flow field in the upstream region is almost unaffected by the flow downstream of the disc because of the high speed ratio of the undisturbed gas.

A cylindrical coordinate system is adopted to describe the region. Advantage may be taken of flow symmetry in order to reduce the number of position coordinates. Since the flow is axially symmetric in this case, only two coordinates i.e. axial and radial, need be stored for each molecule. All locations in azimuthal angle are equally likely. The three velocity components in the coordinate system must be stored for each molecule, because collisions must be calculated as three dimensional phenomena. Note that, because a position radius is stored a change in its direction must be accompanied by an appropriate rotation of the reference frame for the velocity components as well.

The simulated region of physical space is considered as a thin slice of the real space and is divided into a network of cells. Fig. 5.2 shows the region and the cells.

### 5.3 Initial Data

The simulated region is divided into 90 cells. The size of the cells  $\Delta r$  and  $\Delta x$  away from the disc are set equal to the mean free path  $\lambda_\infty$  in the undisturbed gas and those near the disc are set equal to  $\lambda_\infty/2$ . The Knudsen number based on the radius of the disc and the mean free path in the undisturbed gas is chosen as unity, therefore, the size of the disc is automatically fixed. The number of simulated molecules initially distributed in each cell varies from 2 to 10, depending upon the increase in density at the final state so that the variations in sample size are minimized.

Linear dimensions and flow properties are nondimensionalized as follows:

distance	$x$	$x/\lambda_\infty$
velocity	$u$	$u/c_{m_\infty}^* = u\beta_\infty$
time	$t$	$t/(\beta_\infty\lambda_\infty)$
temperature	$T$	$T/T_\infty$
density	$\rho$	$\rho/\rho_\infty$
number density	$n$	$n/n_\infty$
number flux	$N$	$N/(n_\infty/\beta_\infty)$
pressure	$p$	$p/(\rho_\infty/\beta_\infty^2)$
heat flux	$q$	$q/(\rho_\infty/\beta_\infty^3)$

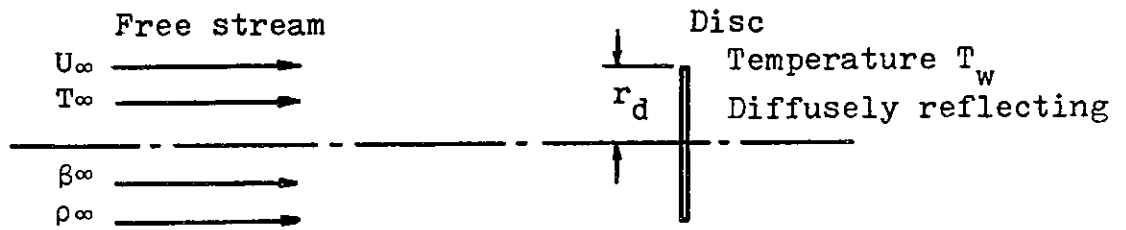


FIG. 5.1 Circular disc in the flow

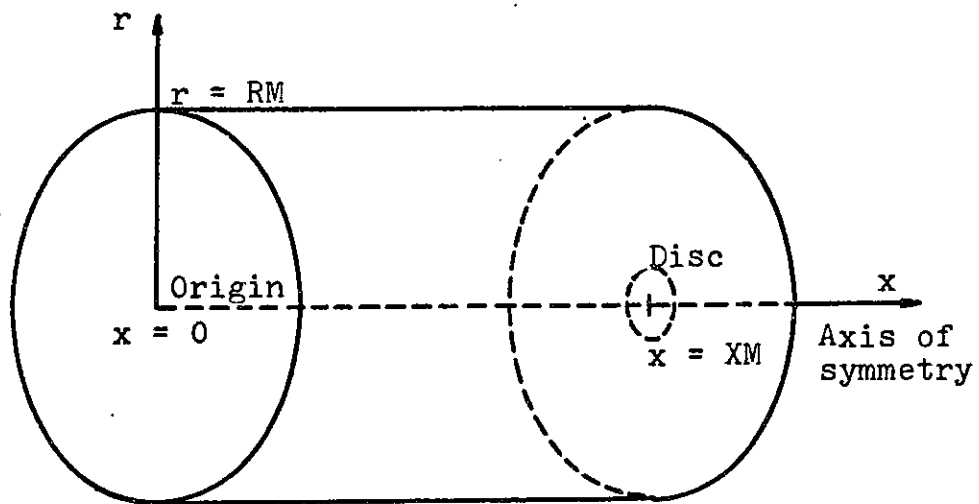


FIG. 5.2 Simulated region of flow field

where

$\lambda_{\infty}$  is the mean free path in the undisturbed gas

$c'_{m_{\infty}}$  is the most probable thermal speed in the undisturbed gas

$\beta_{\infty}$  is the reciprocal of  $c'_{m_{\infty}}$

$T_{\infty}$  is the temperature of the undisturbed gas

$\rho_{\infty}$  is the density of the undisturbed gas

$n_{\infty}$  is the number density of the undisturbed gas

and  $m$  is the mass of molecule

The most probable molecular speed in the undisturbed gas  $c'_{m_{\infty}}$  and its reciprocal  $\beta_{\infty}$  are effectively regarded as having unit value within the program. The mean free path in the undisturbed gas  $\lambda_{\infty}$  is similarly regarded as unity. The undisturbed gas temperature  $T_{\infty}$  and the mass of molecule  $m$  are also regarded as having unit value, so that the Boltzmann constant  $k$  and the gas constant  $R$  are both effectively equal to one half.

#### 5.4 Computational Procedure

The FORTRAN program consisting of a main program MCATD1 and a subroutine FINDCELL2 used for this work is listed as Appendix B.

#### FORTRAN Variables

We consider a gas of hard-sphere molecules uniformly distributed within the simulated region formed by upstream.

$x = 0$  and downstream  $x = XM$  boundaries, a boundary at a radial distance  $RM$ , from axis of symmetry and two surfaces of symmetry with some arbitrary angle between them. This angle is conveniently set equal to  $2$ , so that the area of the disc involved in the simulated region may be fixed to unity. All of the cells are denoted by the subscripts  $(I,J)$ . Fig. 5.3 shows the region.

At time zero, the disc of radius  $DD$  and temperature  $TW$  is instantaneously inserted normal to the flow direction at the downstream edge  $XM$  of the simulated region. The number of simulated molecules  $MC(I,J)$  distributed initially in cell  $(I,J)$ , cell size  $CHX(I,J)$  and  $CHR(I,J)$ , volume  $VL(I,J)$  and weighting factor  $W(I,J)$  are read in as data. The time interval  $\Delta t_m$  is also read in as a data and is stored as  $DTM$ . The integers  $NST$  and  $NIS$  set the other times as multiples of  $\Delta t_m$ : the sampling interval being  $\Delta t_s = NIS * DTM$  and the one data cycle time  $\Delta t_L = \Delta t_s * NST$ .  $NSAM$  denotes the number of total data cycles. The data taken over  $NON$  cycles will not be accepted as a part of the steady state solution. The flow field properties are sampled at time intervals  $\Delta t_s$ , while the surface properties are sampled over these intervals. Again, those properties are not sampled until some time after the start of the program which is defined by the parameter  $NON$ .

The two dimensional array  $P(L,N)$  is used for the storage of the necessary information on the simulated molecules. The subscript  $N$  may be regarded as the molecule number and it is these numbers that are arranged in order of the cells in the cross-referencing array  $LCR(N)$ , which also has the dimension

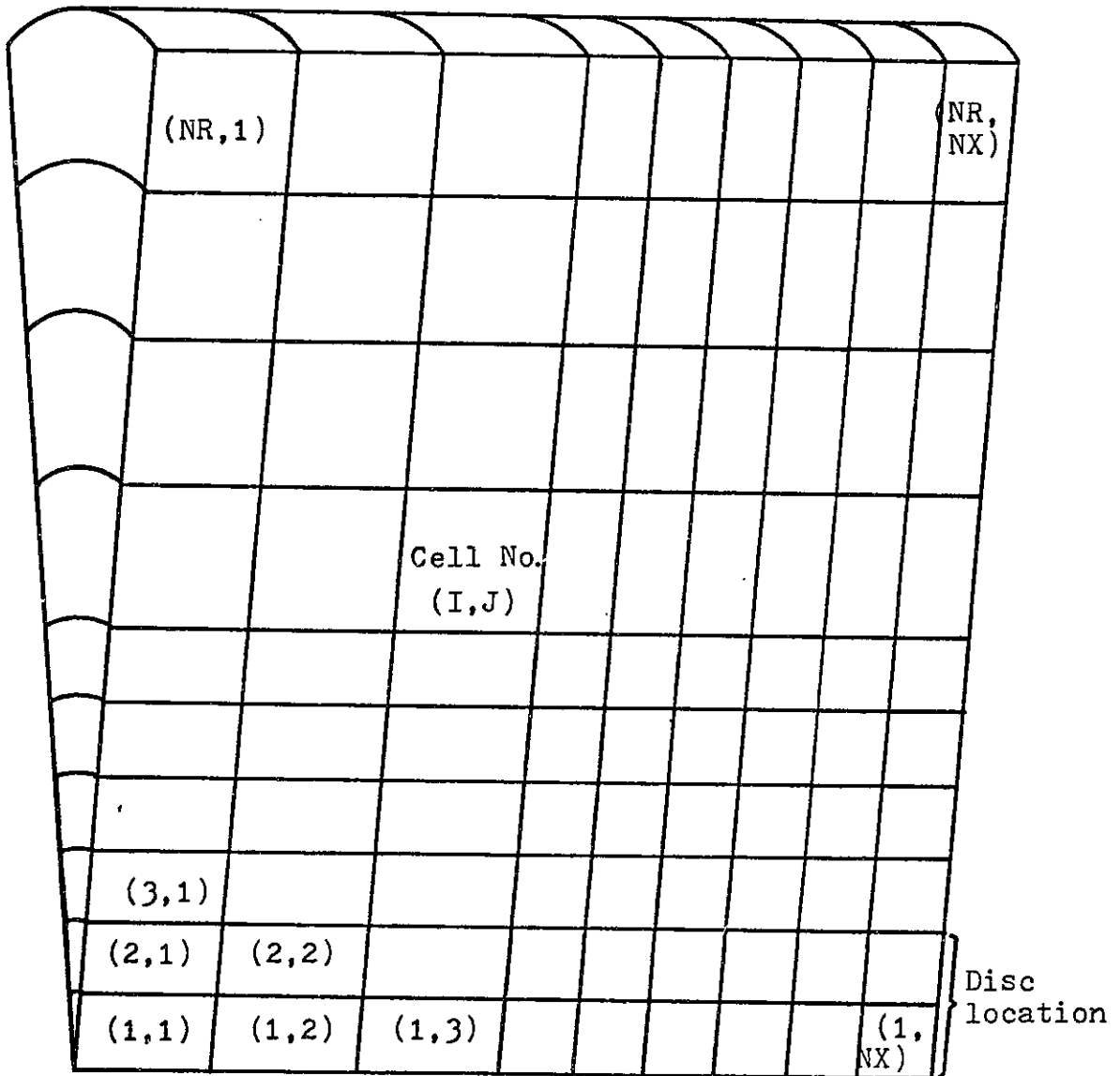


FIG. 5.3 Simulated region and network of cells

N. Since the number of the molecules involved in the flow region varies with time, the dimension N is taken larger having enough margin compared with the actual number of molecules. The subscript L ranges from 1 to 5, with the velocity components in the x, r and  $\theta$  directions being stored in L=1 to 3, respectively. Because of the symmetry of the flow, only the position coordinates x and r need be retained and stored in P(4,N) and P(5,N), respectively.

Since the weighting factors are used, molecules are sometimes removed or duplicated in the cells. The array IP(N) is required in order to distinguish those duplicated molecules from others for the systematic handling of the molecules. The subscript N has the same dimension as in the array P(L,N). A molecule has been duplicated if IP(N)=-1. Otherwise IP(N)=1. The value is reset for each  $\Delta t_m$ .

The starting address of the molecules of cell (I,J) in LCR array is equal to IC(2,I,J)+1 and the number of molecules in the cell is stored in IC(1,I,J). The cell time and the maximum relative speed of cell (I,J) are stored in the arrays C(1,I,J) and C(2,I,J), respectively. They are used for the calculation of collisions. The array SS(K,NN) is required to accumulate and store the samples of the surface properties with the subscript K ranging from 1 to 8 and NN from 1 to 5. The array SC(K,I,J,NN) is used for sampling of the flow field information with K ranging from 1 to 7 and NN from 1 to 5.

The program is for hard sphere molecules, and eqn (3.28) shows that the mean free path in the undisturbed equilibrium



gas is given by

$$\lambda_{\infty} = (2^{\frac{1}{2}} \sigma_T n_{\infty})^{-1} \quad (5.2)$$

Since the normalization procedure defined in section 5.3 sets  $\lambda_{\infty}$  as unity, the collision cross section  $\sigma_T$  is equal to

$$\sigma_T = 1/(2^{\frac{1}{2}} n_{\infty}) \quad (5.3)$$

and is stored as CXS. The average relative speed of collision pairs in the undisturbed gas follows from eqn (3.25) and is stored as VRM.

#### Set Initial State

The coordinates of the initially distributed molecules are calculated. The probability of radial distance is proportional to the distance and  $P(5,N)$  is calculated using eqn (A.8). The x-coordinate  $P(4,N)$  is generated through eqn (A.7). The v and w velocity components of the molecules are generated through eqns (A.18) to (A.20). The thermal velocity component in the x direction is generated through eqns (A.13) and (A.14), and the u velocity component is obtained by adding the free-stream velocity UW to it.

The cell time  $C(1,I,J)$  is set equal to a random fraction of the mean time interval that would be added to them for a collision in the undisturbed gas. The use of this quantity instead of zero makes allowance for the fact that there must

be an integer number of collisions over each DTM and that collisions are calculated until  $C(1,I,J)$  exceeds DTM. The initial approximation to the maximum relative speed in each cell is set, in  $C(2,I,J)$ , to twice the average relative collision speed in the undisturbed gas.

#### Initiate Time

Three DO loops over  $\Delta t_m$ ,  $\Delta t_s$  and  $\Delta t_L$  are set, the second and the third are the multiples of  $\Delta t_m$  through integers NIS and NST, respectively. The inward flux across the upstream boundary appropriate to DTM is calculated. The axial velocity component of the incoming molecules are generated through eqns (A.16) and (A.17), while the other two components are generated through eqns (A.18) to (A.20).

Then all the molecules are moved in the x and r directions over DTM, while for the molecules in the inward flux the time interval DTA is set to random fraction of DTM to avoid the unreasonable distribution near the boundary. Since a radius is stored, a change in its direction must be accompanied by an appropriate rotation of the reference frame for the velocity components. If a molecule is at radius  $r_1$  with velocity components  $v_1$  and  $w_1$ , and moves for time  $\Delta t$ , the new radius is

$$r = \{(r_1 + v_1 \Delta t)^2 + (w_1 \Delta t)^2\}^{1/2} \quad (5.4)$$

Also, the v and w velocity components must be rotated so that v remains the radial component. The new values of v and w are

$$v = \{v_1(r_1 + v_1 \Delta t) + w_1^2 \Delta t\}/r \quad (5.5)$$

and

$$w = w_1 \frac{r_1}{r} \quad (5.6)$$

The calculated new coordinates are stored as X and R. The old coordinates are stored as X1 and R1.

If  $X < 0$ , the molecule is simply considered to be lost. If X is greater than XM, two possibilities must be considered. One is that the molecule simply moves out the region and again the molecule is considered to be lost. The other is that the molecule strikes the disc. The molecule has struck the disc wall if r-coordinate at  $x=XM$  is less or equal to the disc radius DD. In this case, the sampling variables for incident number, normal momentum, parallel momentum and energy are advanced by the appropriate amounts. The v and w components of the reflected molecular velocity may again be generated through eqns (A.18) to (A.20), although  $1/\beta$  is now equal to VMW instead of unity. The distribution function for a velocity component normal to a diffusely reflecting surface follows from eqns (3.43) and (3.44). The distribution of  $u^2$  in eqn (3.44) is identical to the distribution of  $r^2$  that leads to eqn (A.20) so that the post-reflection value of u is  $u = \{-\ln(R_f)\}^{1/2}/VMW$ . The amount of the time interval DTM that remains after the surface interaction is calculated from geometrical consideration

as DTR, and the molecule is moved again appropriate to the reflected velocity components and DTR. The sampling variables for the reflected properties are then advanced.

If  $R$  is greater than  $RM$ , the molecule has moved out the region and the new molecule with the properties in the translating equilibrium gas is generated, so that the net flux across this boundary can be maintained at zero. The velocity components are generated through eqns (A.16) and (A.17) with  $s_n = 0$ , but subject to the condition that  $\beta u_n'$  (or  $\beta v$ , in this case) must be negative. The time interval over which the molecule is moved is set to a random fraction of DTM. The new coordinates are stored as  $R$  and  $X$ .

#### Change in Number of Simulated Molecules

Since the weighting factor is used in the present program the provision has to be made for a systematic change in number of molecules if molecules cross the cell boundary. The cell numbers for old and new coordinates are calculated using the old and new coordinates ( $R_1, X_1$ ) and ( $R, X$ ) respectively, by the subroutine FINDCELL2 as ( $I, J$ ) and ( $K, L$ ), respectively. The number of molecules in the new cell should be equal to  $W(I, J) / W(K, L)$  and, since this is generally not an integer, the removal or duplication is based on an acceptance-rejection method. The routine can best be deduced from the coding which contains 15 lines starting from label 35.

#### Molecular Indexing

The molecular indexing information in the arrays LCR(N) and IC(2, I, J) is not used prior to the collision calculation

routine and is most conveniently set between the molecular motion and collision calculation of the program. The procedure for this necessarily samples the number of molecules per cell and, therefore, the number density. The number density is the only macroscopic quantity required by collision calculation. This algorithm is again best deduced directly from the coding between labels 60 and 65. Subroutine FINDCELL2 is used to determine the cell number (I,J) directly from the position coordinates (P(5,N), P(4,N)) of a molecule.

#### Calculate Collisions

Appropriate number of collisions are calculated in each cell. No collisions are calculated unless the number of molecules in the cell is greater or equal to 2. The numbers of the molecules in cell (I,J) are stored in the cross reference array LCR(N) for value of N between IC(2,I,J)+1 and IC(2,I,J)+IC(1,I,J). One molecule is selected randomly among those molecules. A second molecule is then selected in a similar way to constitute a possible collision pair as long as these two molecules are different. The relative speed VR between these two molecules is calculated from three velocity components of the molecules. Since the probability of collision is proportional to the relative speed VR, the collision pair is retained or rejected on this basis using the acceptance-rejection method. If the pair is retained the collision time interval for the collision is calculated from eqn (4.2) and is added to the cell time counter C(1,I,J). The collision counter SC(7,I,J) is advanced by one for each collision.

The post collision velocity components are generated through eqns (3.10) and (4.3).

These steps are repeated until the cell time counter  $C(1,I,J)$  exceeds the overall flow time TIME.

#### Sample Flow Properties

At the sampling intervals  $\Delta t_s = NIS \cdot \Delta t_m$ , the sample size  $\Sigma N$ ,  $\Sigma u$ ,  $\Sigma v$ ,  $\Sigma u^2$ ,  $\Sigma v^2$  and  $\Sigma w^2$  are sampled, and are stored in the array from  $SC(1,I,J,NN)$  to  $SC(6,I,J,NN)$ . They are accumulated over the one data cycle  $\Delta t_L = NST \cdot \Delta t_s$ . At the end of the time interval  $\Delta t_L$ , the sampled information is put into the required form and printed. The flow properties are calculated from the information stored in the SC array. The normalized density in each cell is obtained by dividing  $\Sigma N$  by the product of the time multiplicative NST and the number of molecules per cell  $MC(I,J)$  in the undisturbed gas. The average velocities in x and y directions are simply  $\bar{u} = (\Sigma u) / (\Sigma N)$  and  $\bar{v} = (\Sigma v) / (\Sigma N)$ , respectively. The kinetic temperature  $T_x$  based on the u component of the velocity is given from the relation

$$\frac{1}{2} k T_x = \frac{1}{2} m \overline{u^2} = \frac{1}{2} m (\overline{u^2} - \bar{u}^2)$$

Thus we have

$$T_x = \frac{m}{k} (\overline{u^2} - \bar{u}^2) = \frac{m}{k} \{ (\Sigma u^2) / (\Sigma N) - \bar{u}^2 \}$$

or, noting our normalization

$$T_x = 2 \{ (\Sigma u^2) / (\Sigma N) - \bar{u}^2 \} \quad (5.7)$$

The other kinetic temperatures  $T_r$  and  $T_\theta$  are obtained in a similar manner, although  $\bar{w}$  is zero for  $T_\theta$ . The temperature is obtained as the mean of the three temperature components.

$$T = \frac{1}{3} (T_X + T_r + T_\theta) \quad (5.8)$$

The surface properties are based on the sampled flux of molecular number, momentum and energy incident on and reflected from the surface. Since the multiplicative factor for the velocity components in the normalization is effectively unity, the required nondimensional fluxes are obtained by dividing the sums of the appropriate quantities by the product of the total time interval and the undisturbed number density.

## CHAPTER 6

### RESULTS AND DISCUSSION

#### 6.1 Flow Properties

The computation was carried out for a flow of speed ratio ten with the surface temperature of the disc equal to the freestream temperature. The knudsen number is unity and the corresponding Reynolds number based on freestream conditions and the disc radius is  $Re_{\infty} = 17.7$ . In the definition, the viscosity coefficient is taken as

$$\mu_{\infty} = \frac{1}{2} \rho_{\infty} \bar{c}'_{\infty} \lambda_{\infty}$$

and is proportional to  $T^{1/2}$ .

#### Flow Field

Information was obtained at a number of discrete positions representing the cells in the flow field on the value of the directed velocity, the local density and the local temperature. Figures 6.1 to 6.3 illustrate the changes that occur in these flow quantities. The density and the temperature are indicated by contour lines which are interpolated between the sampled properties at discrete points. The directed velocities are indicated by lines of the appropriate length and direction. The distance from the stagnation point is normalized with respect to the radius of the disc.



The near-axis density, velocity, temperature and the kinetic temperature based on the thermal velocities in the particular directions are presented in Figures 6.4 to 6.7. Also shown in the figures are the Rankine-Hugoniot conditions for comparison.

The temperature disturbance seems to extend far from the disc, although the disturbed region in terms of the density and the velocity is confined to comparatively small region. There is no physical explanation why the temperature disturbance is decoupled from others to such extent. This is probably caused by the high speed ratio. If

$$E = \frac{1}{2} mc^2 + \frac{3}{2} kT \sim \text{const.}$$

differentiating both sides of the equation, we have

$$mcdc + \frac{3}{2} kdT \sim 0$$

or

$$\frac{dT}{T} \approx -\frac{2}{3} \frac{c^2}{RT} \frac{dc}{c}$$

But for the flow region away from the disc

$$\frac{c^2}{2RT} \approx S^2 \sim 100$$

Thus we have

$$\frac{dT}{T} \sim -133 \frac{dc}{c}$$

in the region away from the disc. Therefore, a 50% change in  $T$  corresponds to a 0.4% change in  $c$  which may not be detectable. This effect would have been much less if  $T$  behind the shock had been used to normalize the temperature. Further, we should expect temperature fluctuations to be much larger than velocity (or density) fluctuations, as can be clearly seen from eqn (5.7), from which the temperature is calculated.

### Surface Interaction

Figure 6.8 illustrates the average heat transfer rate to the surface in terms of the Stanton number which is defined by

$$St = \frac{q}{\rho_{\infty} U_{\infty} (H_o - H_w)} \quad (6.1)$$

In the figure, the Stanton number  $St$  is normalized by the free-stream value  $St_{fm}$  which can be obtained analytically through eqn (3.51). Also shown in this figure are the heat transfer rate to a sphere and cylinder obtained by Bird [1] and to a bluff-faced cylinder obtained by Pullin et al [24]. It is reasonable for the present result to take a slightly higher value than the result by Pullin et al, because the wall temperature is lower and the freestream velocity is larger in our case.

Figure 6.9 shows the drag coefficient data. In the calculation of the drag coefficient from the pressure data output, it has been assumed that the pressure on the rear side of the disc is zero. The data is also normalized by the free molecule value obtained through eqn (3.49).

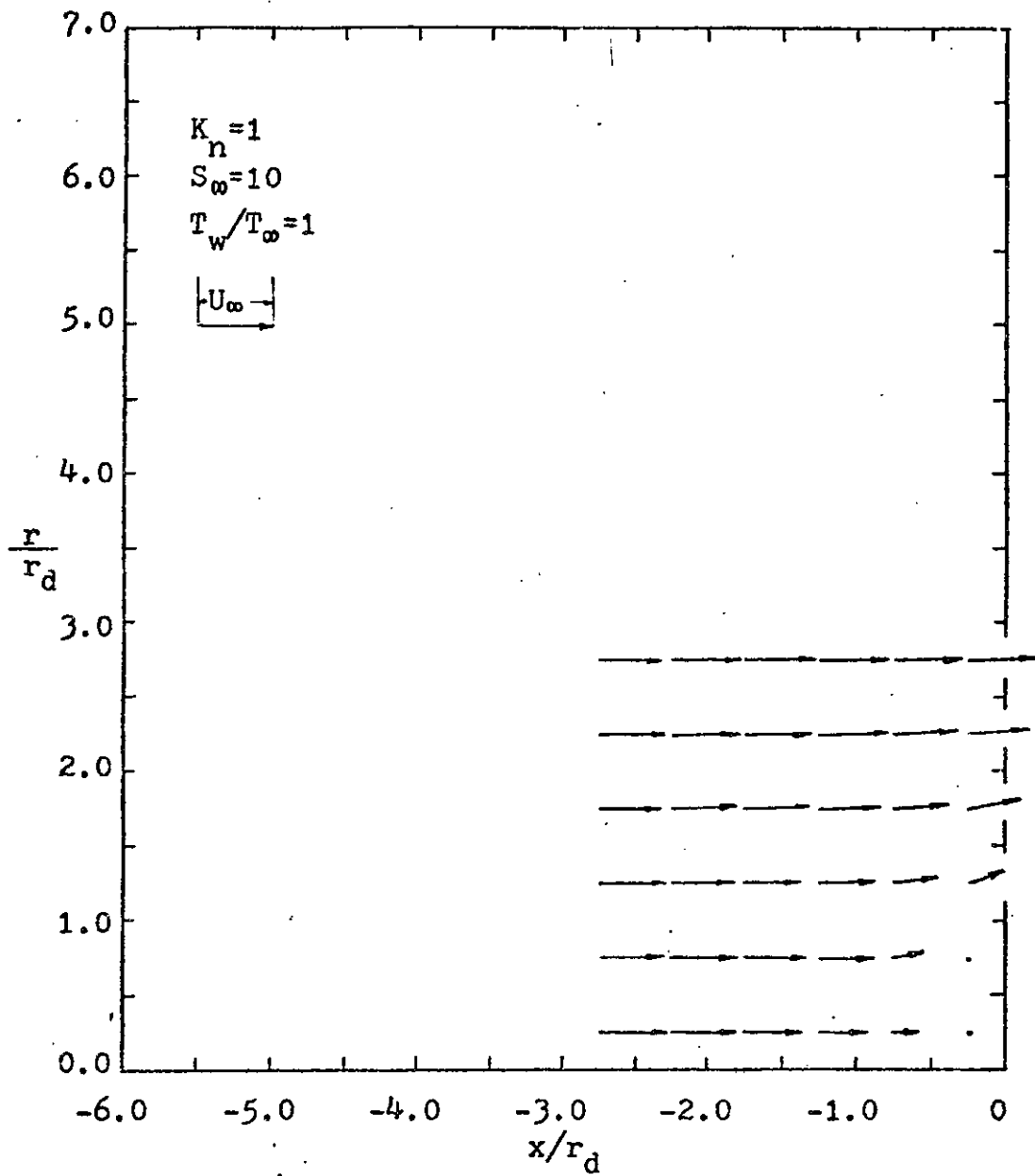


FIG. 6.1 Directed velocities

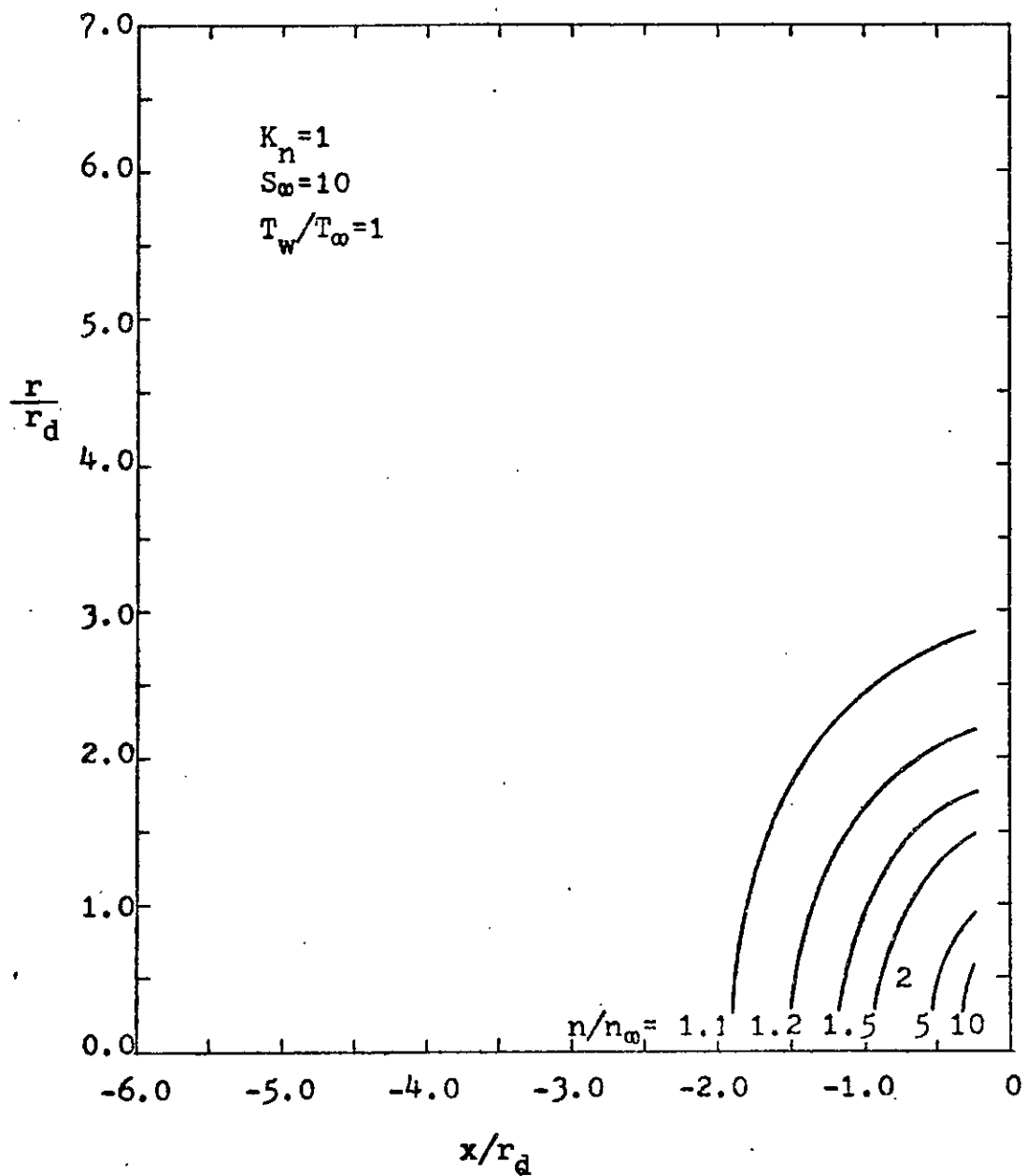


FIG. 6.2 Density contours

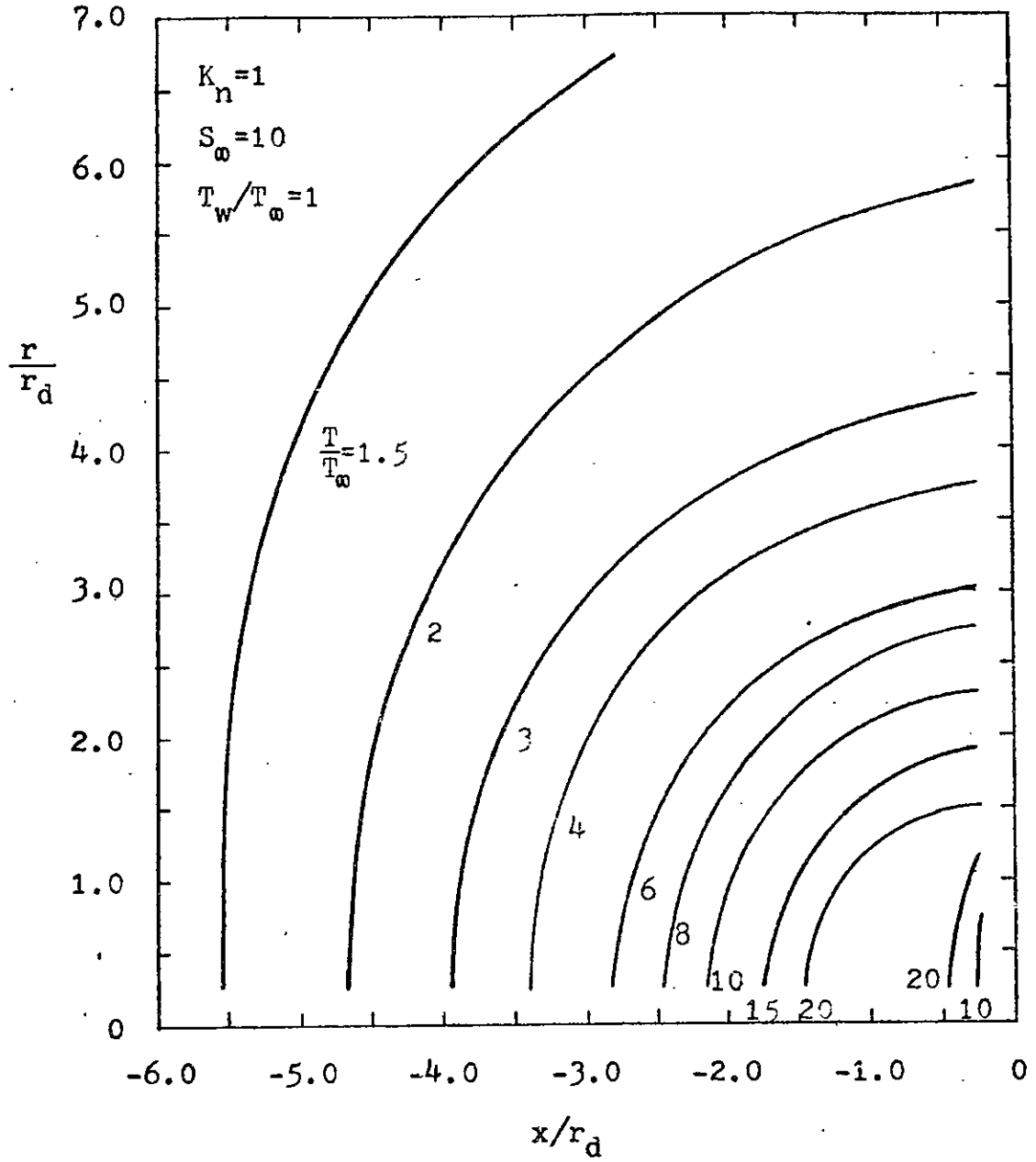


FIG. 6.3 Temperature contours

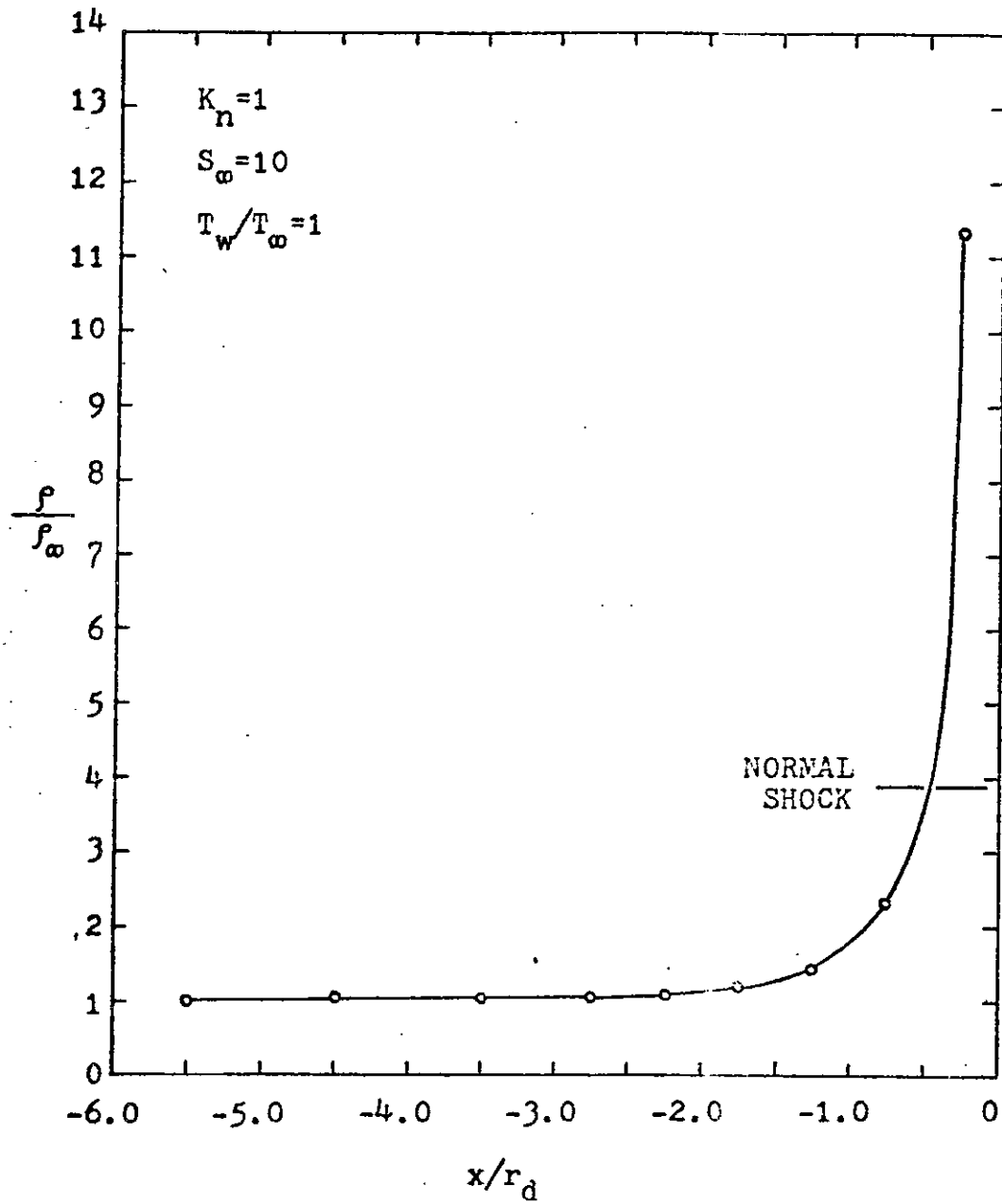


FIG. 6.4 Near axis density profile

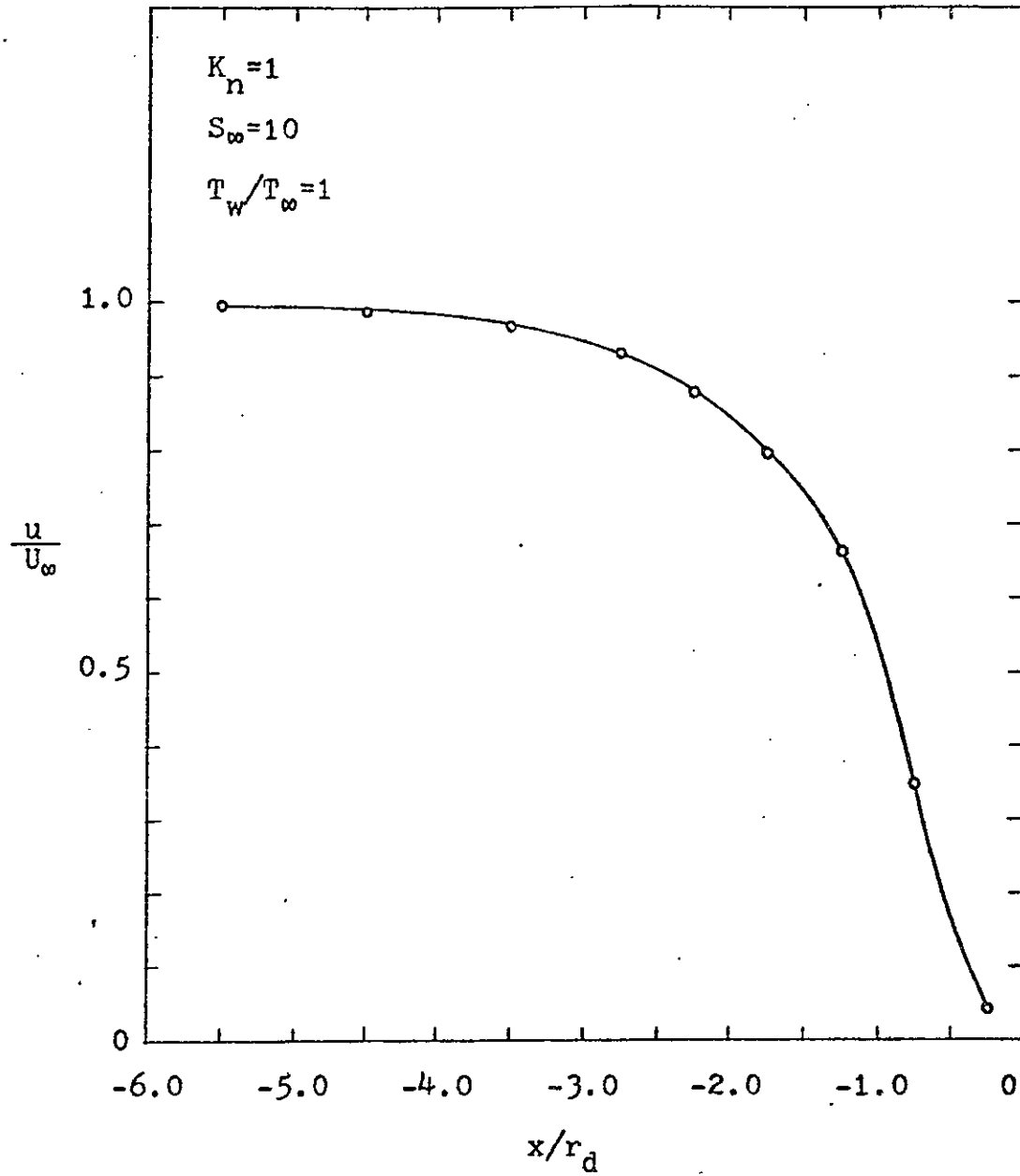


FIG. 6.5 Near axis streamwise velocity profile

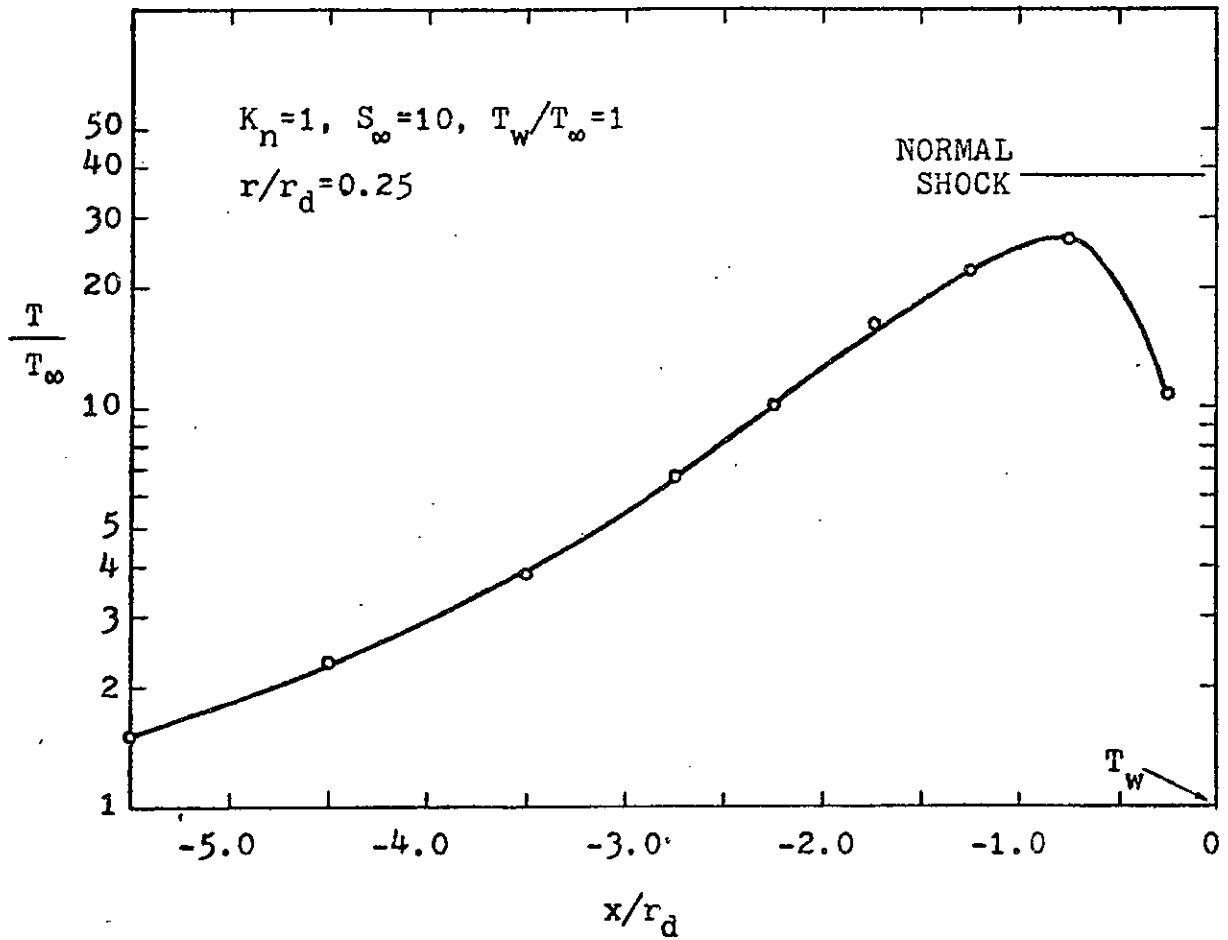


FIG. 6.6 Near axis temperature profile



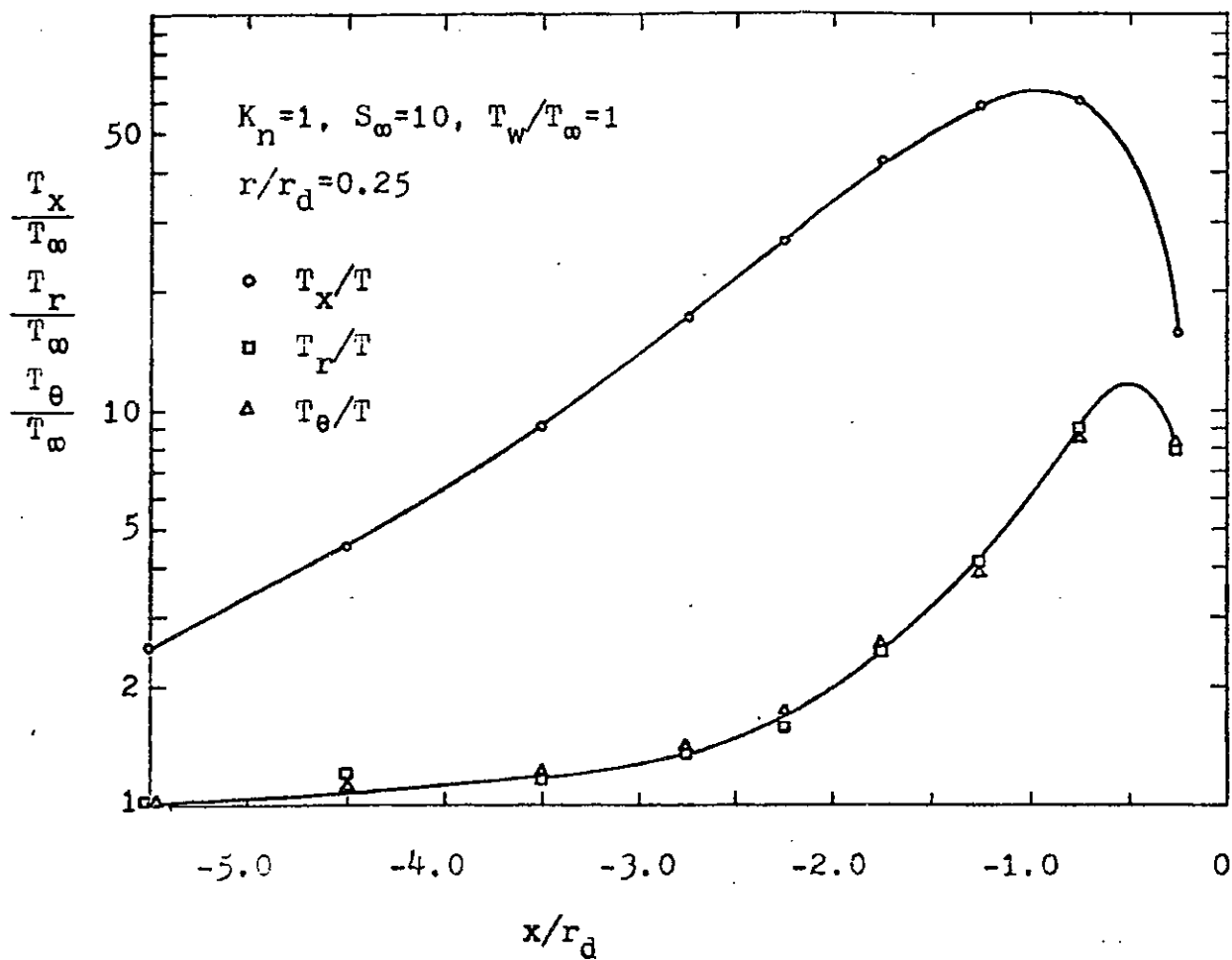


FIG. 6.7 Near axis kinetic temperature profiles

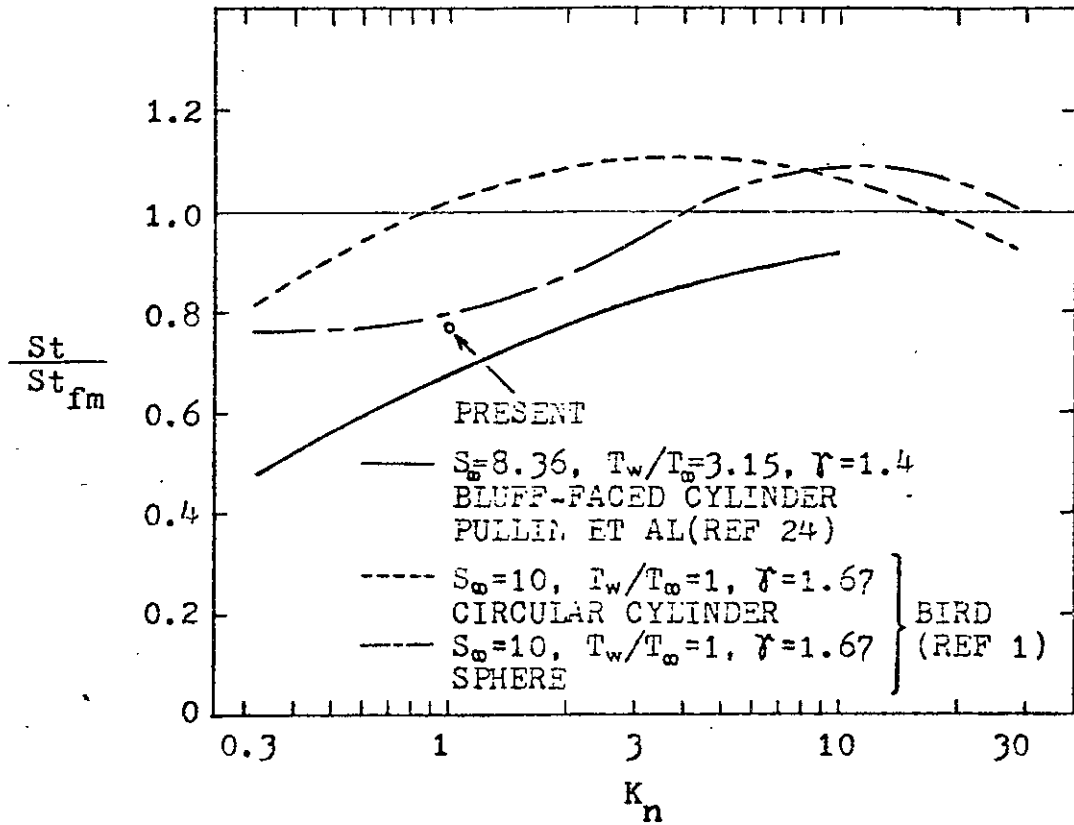


FIG. 6.8 Average heat transfer rate

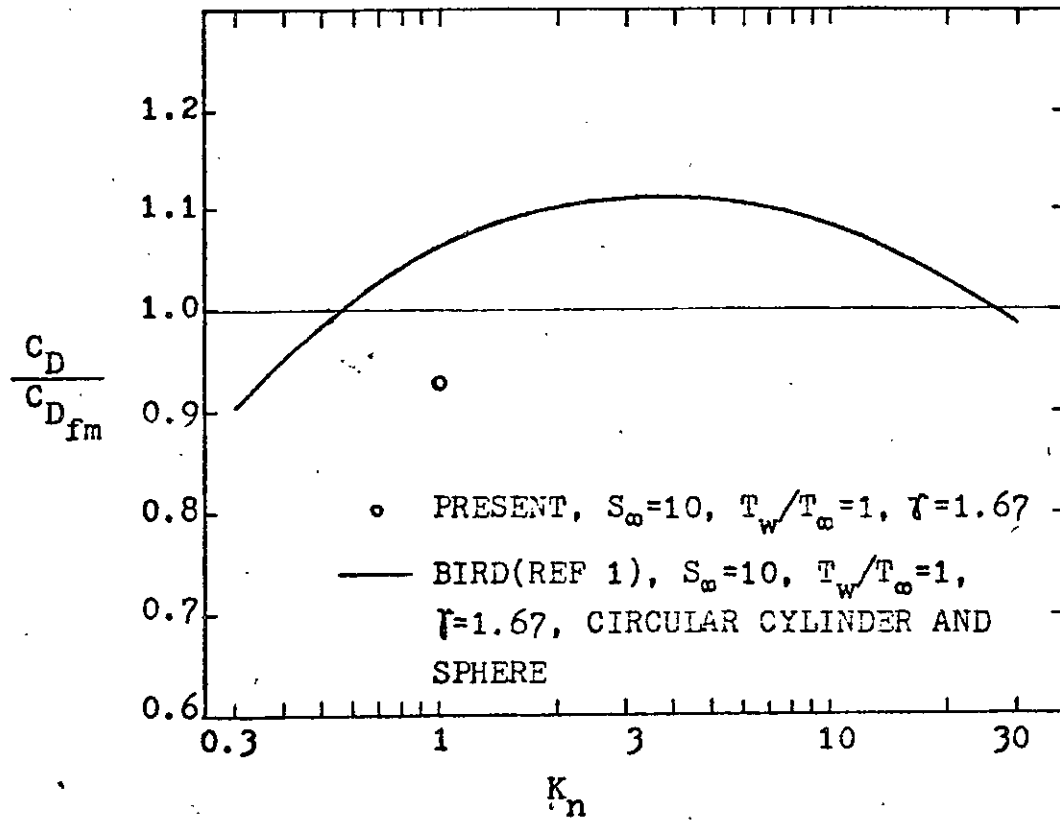


FIG. 6.9 Drag coefficient

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## APPENDIX A

## SELECTION OF RANDOM EVENTS

The essential feature of the Monte Carlo method is probabilistic modelling of real physical process in which variables are distributed in a prescribed manner. The method requires the generation of representative values of the variates. This is done through random numbers.

A.1 Random Numbers

Random numbers are generated by the function called Pseudo-Random Number RAN (I1,I2) supplied by the VAX/VMS VOL as a standard subprogram.

Format : RAN (I1,I2)

Arguments: I1, I2

Integer \*2 variables or array elements that contain the seed for computing the random numbers.

Notes : 1. The values of I1 and I2 are updated during the computation to contain the updated seed.

2. The algorithm for computing the random number value is as follows:

If I1=0 and I2=0, set generator base

$$x(n+1)=2^{**}16+3 \quad (\text{A.1})$$

Otherwise

$$x(n+1)=(2^{**}16+3)*x(n)\text{mod}2^{**}32 \quad (\text{A.2})$$

Store generator base x(n+1) in I1,I2.

Result is  $x(n+1)$  scaled to a real value  
 $Y(n+1)$ , for  $0.0 \leq Y(n+1) \leq 1.0$ .

## A.2 Sampling From a Prescribed Distribution

If a variable  $x$  follows a random process, the distribution of the variable may be prescribed by a normalized distribution function such that a probability of a value lying between  $x$  and  $x+dx$  is given by

$$f_x dx \quad (A.3)$$

If the range of  $x$  is from  $a$  to  $b$ , then the total probability is

$$\int_a^b f_x dx = 1 \quad (A.4)$$

The cumulative distribution function is defined as

$$F_x = \int_a^x f_x dx \quad (A.5)$$

A random fraction  $R_f$  will now be generated and be set equal to  $F_x$ . The representative value of variate  $x$  is given by

$$F_x = R_f \quad (A.6)$$

## A.3 Distribution Functions

We now consider the cases which appear in the main text of this paper.

(a) The variate  $x$  is uniformly distributed between  $a$  and  $b$ .

In this case  $f_x = \text{constant}$  and using eqn (A.4)

$$f_x = 1/(b-a)$$

Therefore, from eqns (A.5) and (A.6)

$$F_x = \int_a^x \frac{1}{b-a} dx = (x-a)/(b-a) = R_f$$

or

$$x = a + R_f(b-a) \quad (\text{A.7})$$

(b) The variate  $x$  is distributed so that the probability of  $x$  is proportional to  $x$ .

Using eqn (A.4)

$$f_x = 2x/(b^2 - a^2)$$

From eqns (A.5) and (A.6)

$$F_x = (x^2 - a^2)/(b^2 - a^2) = R_f$$

or

$$x = \{a^2 + R_f(b^2 - a^2)\}^{1/2} \quad (\text{A.8})$$

For a special case where  $a=0$

$$x = b(R_f)^{1/2} \quad (\text{A.9})$$



#### A.4 Acceptance-Rejection Method

Above procedure is applicable only when it is possible to invert eqn (A.6) to obtain an explicit function for  $x$ . This can be handled by acceptance-rejection method. In order to make direct use of random number, distribution function  $f_x$  is divided by its maximum value,  $f_{\max}$ , to give

$$f'_x = f_x / f_{\max} \quad (\text{A.10})$$

A representative value of the variate  $x$  is chosen on the assumption that  $x$  has a rectangular distribution between  $a$  and  $b$ . Eqn (A.7) can be used to give

$$x = a + R_f (b - a) \quad (\text{A.11})$$

The value of  $f'_x$  is calculated for this value of  $x$  and compared with a further generated random fraction,  $R_f$ . If  $f'_x$  is greater than  $R_f$ , the value of  $x$  is accepted. If  $f'_x$  is less than  $R_f$ , the value of  $x$  is rejected and the procedure will be repeated until a value of  $x$  is accepted.

Since  $R_f$  is uniformly distributed between 0 and 1, the probability of  $x$  being accepted is obviously proportional to  $f_x$  and the successive accepted values conform to the distribution.

(a) Consider the distribution function  $f_u$ , for the thermal velocity component in an equilibrium gas.

$$f_u = \frac{\beta}{\pi^{1/2}} \exp(-\beta^2 u'^2) \quad (\text{A.12})$$

The function takes the maximum value  $\beta/\pi^{1/2}$  at  $u'=0$ . Dividing  $f_{u'}$  by the maximum value to get

$$f'_{u'} = \exp(-\beta^2 u'^2)$$

The uniformly distributed value of  $u'$  is calculated by eqn (A.7) with  $a$  and  $b$  set as arbitrary cast-off values instead of the real values  $-\infty$  and  $+\infty$  in order to make this procedure effective. If we take 3 times standard deviation for these values, i.e.,  $-3/\beta$  and  $+3/\beta$  for  $a$  and  $b$  respectively, the fraction lying outside of this range is  $1-\text{erf}(3)$ , or 0.000022. These cast-off values are considered fairly reasonable unless the tail effect is too significant. Therefore, from eqn (A.7)

$$u' = (-3 + 6R_f) / \beta \quad (\text{A.13})$$

and

$$f'_{u'} = \exp\{-(-3 + 6R_f)^2\} \quad (\text{A.14})$$

The next value of  $R_f$  is generated. The value of  $u'$  is accepted if  $f'_{u'} > R_f$ . If  $f'_{u'} < R_f$  the value of  $u'$  is rejected and the procedure is repeated until  $u'$  is accepted.

(b) Consider the distribution function for the thermal velocity component normal to the boundary

$$f_{\beta u'_n} = \frac{1}{\pi^{1/2} \beta} (\beta u'_n + S_n) \exp(-\beta^2 u'^2_n) \quad (\text{A.15})$$

where  $u'_n$  is the thermal velocity component normal to the boundary and  $S_n$  is the stream velocity normal to the boundary.  $f_{\beta u'_n}$  takes its maximum value at  $\beta u'_n = \{(Sn^2+2)^{1/2} - Sn\}/2$  as

$$f_{\max} = \frac{1}{\pi^{1/2} \beta} \left[ \{(Sn^2+2)^{1/2} - Sn\}/2 + Sn \right] \exp \left( -\frac{\{(Sn^2+2)^{1/2} - Sn\}^2}{4} \right)$$

The normalized distribution is

$$f'_{\beta u'_n} = \frac{2(\beta u'_n + Sn)}{Sn + (Sn^2+2)^{1/2}} \exp \left( \frac{1}{2} + \frac{Sn}{2} \{Sn - (Sn^2+2)^{1/2}\} - \beta^2 u'^2_n \right)$$

Adopting the same range as in (a), eqn (A.7) gives

$$\beta u'_n = -3 + 6R_f \quad (\text{A.16})$$

and

$$f'_{\beta u'_n} = \frac{2[(-3+6R_f) + Sn]}{(Sn^2+2)^{1/2} + Sn} \exp \left( \frac{1}{2} + \frac{Sn}{2} \{Sn - (Sn^2+2)^{1/2}\} - (-3+6R_f)^2 \right) \quad (\text{A.17})$$

The next value of  $R_f$  is then generated and, if  $f'_{\beta u'_n} > R_f$  then  $\beta u'_n$  is accepted. If  $f'_{\beta u'_n} < R_f$  the value of  $\beta u'_n$  is rejected and the process is repeated until a value of  $\beta u'_n$  is accepted.

(c) The alternative way is available for a special case. This provides the sampling pairs of values from the normal distribution of eqn (A.12). These values are denoted by  $u'$  and  $v'$  and from eqn (A.12),

$$\begin{aligned} f_{u'} du' f_{v'} dv' &= (\beta/\pi^{1/2}) \exp(-\beta^2 u'^2) du' (\beta/\pi^{1/2}) \exp(-\beta^2 v'^2) dv' \\ &= (\beta^2/\pi) \exp\{-\beta^2 (u'^2 + v'^2)\} du' dv' \end{aligned}$$

Now set

$$u' = r \cos\theta$$

and

$$v' = r \sin\theta \quad (\text{A.18})$$

Then, since the Jacobian

$$\frac{\delta(u', v')}{\delta(r, \theta)} = \begin{vmatrix} \frac{\delta u'}{\delta r} & \frac{\delta u'}{\delta \theta} \\ \frac{\delta v'}{\delta r} & \frac{\delta v'}{\delta \theta} \end{vmatrix} = \begin{vmatrix} \cos\theta & -r \sin\theta \\ \sin\theta & r \cos\theta \end{vmatrix} = r ,$$

$$\begin{aligned} f_{u'} du' f_{v'} dv' &= (\beta^2/\pi) \exp(-\beta^2 r^2) r dr d\theta \\ &= \exp(-\beta^2 r^2) d(\beta^2 r^2) d\theta / 2\pi \end{aligned}$$

The angle  $\theta$  is uniformly distributed between 0 and  $2\pi$  so that, from eqn (A.11)

$$\theta = 2\pi R_f \quad (\text{A.19})$$

The variable  $\beta^2 r^2$  is distributed between 0 and  $\infty$  and its distribution function

$$f_{\beta^2 r^2} = \exp(-\beta^2 r^2)$$

is also already in a normalized form. The cumulative distribution function is

$$F_{\beta^2 r^2} = 1 - \exp(-\beta^2 r^2)$$

and noting that  $R_f$  and  $1-R_f$  are equivalent functions, eqn (A.6) gives

$$r = \{-\ln(R_f)\}^{1/2} / \beta \quad (\text{A.20})$$

A pair of values  $r$  and  $\theta$  may be sampled from eqns (A.19) and (A.20) using successive random fractions. The normally distributed values of  $u'$  and  $v'$  follow from eqn (A.18) and provide typical values for a thermal velocity component in equilibrium gas.

APPENDIX B  
LISTING OF PROGRAMS

Contained herein are the main program MCATD1 and the subroutine program FINDCELL2.

```

PROGRAM MCATD1

DIMENSION C(2,10,10),IC(2,10,10),SC(7,10,10,5),NIM(10),
1 SS(8,5),W(10,10),OP(9),URC(3),CHX(10,10),
1 CHR(10,10),MC(10,10),VL(10,10),P(5,4000),IP(4000),LCR(4000)
READ(3,1) NSAM,NST,NIS,NON,NCR,NCX,NCRI,NCX1,I1,I2
1 FORMAT(10I4)
READ(3,2) RM,XM,DD,UW,TW,FND,DTM,ERFUW
2 FORMAT(5F6.2,3F8.5)
READ(3,3) ((W(I,J),I=1,NCR),J=1,NCX)
3 FORMAT(10F7.3)
READ(3,4) ((MC(I,J),I=1,NCR),J=1,NCX)
4 FORMAT(10I7)
READ(3,5) ((CHR(I,J),I=1,NCR),J=1,NCX)
5 FORMAT(10F7.3)
READ(3,6) ((CHX(I,J),I=1,NCR),J=1,NCX)
6 FORMAT(10F7.3)
READ(3,7) ((VL(I,J),I=1,NCR),J=1,NCX)
7 FORMAT(10F7.3)
WRITE(4,101)
101 FORMAT(' DIRECT MONTE CARLO SIMULATION')
WRITE(4,102)
102 FORMAT(' RAREFIED HYPERSONIC GAS FLOW PAST A CIRCULAR',
1 ' DISC'//)
WRITE(4,103) DD,XM,TW
103 FORMAT(' THE DISC OF RADIUS',F5.2,' AT X=',F5.2,
1 ' IS DIFFUSELY REFLECTING WITH TEMP.',F6.2)
WRITE(4,104) XM,RM
104 FORMAT(' CONTROL VOLUME IS A REGION FORMED BY X=0.0,X=',
1 F5.2,' AND R=',F5.2)
WRITE(4,105) UW
105 FORMAT(' VELOCITY OF UNIFORM FREE STREAM IS UW=',F5.2)
WRITE(4,106) DTM
106 FORMAT(' THE MOLECULES ARE ALLOWED TO MOVE OVER THE',
1 ' TIME PERIOD',F11.7//)
WRITE(4,85)
85 FORMAT(' SURFACE PROPERTIES '//)
WRITE(4,86)
86 FORMAT(' NN SAMPLE SIZE NUMBER FLUX PRESSURE',
1 ' SHEAR STRESS ENERGY FLUX')
WRITE(4,87)
87 FORMAT(' NONWTD WTD WTD INCIDENT ',
1 ' REFLECTED INCIDENT REFLECTED INCIDENT REFLECTED')
C SET CONSTANTS
PI=3.141593
VMW=SQRT(TW)

```

```

      CXS=1./ (SQRT(2.)*FND)
      VRM=2.*SQRT(2./PI)
      DO 13 NN=1,5
      SS(B,NN)=0.
      DO 13 M=1,7
      SS(M,NN)=0.
      DO 13 J=1,NCX
      DO 13 I=1,NCR
13      SC(M,I,J,NN)=0.
      BB=SQRT(UW*UW+2.)
      A=1.+ERFUW
      FX1=(MC(1,1)*DTM/CHX(1,1))*(EXP(-1/UW*UW)+SQRT(PI)*UW*A)/
      1 (2.*SQRT(PI))
      FX2=FND*NCX*CHX(NCR,1)*DTM*RM/(W(NCR,1)*DD*DD*SQRT(PI))
      C INITIAL STATE WILL NOW BE SET
      N=0
      X2=0.
      DO 19 J=1,NCX
      R2=0.
      X1=X2
      X2=X1+CHX(1,J)
      DO 19 I=1,NCR
      C(1,I,J)=2.*RAN(I1,I2)/(MC(I,J)*CXS*FND*VRM)
      C(2,I,J)=2.*VRM
      R1=R2
      R2=R1+CHR(I,J)
      DO 18 K=1,MC(I,J)
      N=N+1
      P(4,N)=X1+(X2-X1)*RAN(I1,I2)
      P(5,N)=SQRT((R2*R2-R1*R1)*RAN(I1,I2)+R1*R1)
17      A=-3.+6.*RAN(I1,I2)
      B=2.*(A+UW)*EXP(0.5+0.5*UW*(UW-BB)-A*A)/(UW+BB)
      BBB=RAN(I1,I2)
      IF(B,LT,BBB) GO TO 17
      P(1,N)=UW+A
      B=SQRT(-ALOG(RAN(I1,I2)))
      A=2*PI*RAN(I1,I2)
      P(2,N)=B*COS(A)
      P(3,N)=B*SIN(A)
      IF(N)=1
18      CONTINUE
19      CONTINUE
      NM=N
      C INITIATE TIME
      DO 81 NN=1,NSAM
      DO 83 JJ=1,NST
      DO 80 II=1,NIS
      TIME=((NN-1)*NST+(JJ-1))*NIS+II)*DTM
      C INWARD FLUX THROUGH X=0.
      K=FX1
      B=FX1-1.*K
      NM2=0
      DO 14 I=1,NCR
      A=RAN(I1,I2)
      K=FX1
      IF(B.GT,A) K=K+1
      NIM(I)=K
14      NM2=NM2+NIM(I)
      K=NM
      NM=K+NM2
      DO 21 I=1,NCR
      DO 21 J=1,NIM(I)
      K=K+1
      P(4,K)=0.
      A=RAN(I1,I2)
      IF(I.GE,NCR1) GO TO 16

```



```

P(5,K)=CHR(1,1)*SQRT((2*I-1)*A+(I-1)*(I-1))
GO TO 15
16 P(5,K)=CHR(NCR1,1)*SQRT((2*I-7)*A+(I-4)*(I-4))
15 AA=-3.+6.*RAN(I1,I2)
A=AA+UW
IF(A.LT.0.) GO TO 15
B=2.*A*EXP(0.5+0.5*UW*(UW-BB)-AA*AA)/(UW+BB)
BBB=RAN(I1,I2)
IF(B.LT.BBB) GO TO 15
P(1,K)=A
B=SQRT(-ALOG(RAN(I1,I2)))
A=2.*PI*RAN(I1,I2)
P(2,K)=B*COS(A)
P(3,K)=B*SIN(A)
IP(K)=1
21 CONTINUE
C MOVE MOLECULES
30 N=0
24 N=N+1
IF(N.GT.NM) GO TO 60
IF(IP(N).LT.0) GO TO 24
X1=P(4,N)
R1=P(5,N)
P2=P(2,N)
P3=P(3,N)
C ABOVE ARE OLD COORDINATES
IF(X1.EQ.0.) GO TO 25
C E-MOLECULES
X=X1+P(1,N)*DTM
R=SQRT((R1+P2*DTM)*(R1+P2*DTM)+P3*P3*DTM*DTM)
P(2,N)=(P2*(R1+P2*DTM)+P3*P3*DTM)/R
P(3,N)=P3*R1/R
GO TO 26
C I-MOLECULES
25 DTA=RAN(I1,I2)*DTM
IF(DTA.LT.1.E-10) DTA=1.E-10
X=X1+P(1,N)*DTA
R=SQRT((R1+P2*DTA)*(R1+P2*DTA)+P3*P3*DTA*DTA)
P(2,N)=(P2*(R1+P2*DTA)+P3*P3*DTA)/R
P(3,N)=P3*R1/R
C ABOVE ARE NEW COORDINATES
26 IF(X.LT.0.) GO TO 54
IF(X.GT.XM.AND.R.GT.RM) GO TO 300
IF(X.GT.XM) GO TO 27
IF(R-RM) 35,35,301
300 RRM=(R-R1)*(XM-X1)/(X-X1)
IF(RRM.LT.RM) GO TO 54
C MOLECULE IS COMING INTO C.V. THROUGH THE BOUNDARY R=RM
301 A=3.*RAN(I1,I2)
B=SQRT(2.)*A*EXP(0.5-A*A)
BBB=RAN(I1,I2)
IF(B.LT.BBB) GO TO 301
P(2,N)=-A
302 B=SQRT(-ALOG(RAN(I1,I2)))
A=2.*PI*RAN(I1,I2)
P(1,N)=UW+B*COS(A)
P(3,N)=B*SIN(A)
DTA=DTM*RAN(I1,I2)
R=SQRT((RM+P(2,N)*DTA)*(RM+P(2,N)*DTA)+
1 P(3,N)*P(3,N)*DTA*DTA)
IF(R.GT.RM) GO TO 302
X=XM*RAN(I1,I2)
GO TO 35
27 RD=R-(R-R1)*(X-XM)/(X-X1)
C RD IS A COORD. OF THE MOLECULE AT X=XM
IF(RD.GT.DD) GO TO 54

```

```

C THE MOLECULE STRIKES DISC
C DISC HAS DIFUSELY REFLECTING SURFACE
  ITR=DTM*(X-XM)/(X-X1)
C DTR IS TIME REMAINING AFTER THE MOLECULE STRIKES DISC
  IF(DTR.LT.1.E-10) DTR=1.E-10
  DTH=DTM-DTR
  VD=(P2*(R1+P2*DTH)+P3*P3*DTH)/RD
  WD=P3*R1/RD
C SAMPLING WILL NOT BE DONE UNLESS MM IS POSITIVE
  MM=NN-NON
  IF(MM.LE.0) GO TO 33
  CALL FINDCELL2(R1,X1,I,J)
  SS(1,MM)=SS(1,MM)+W(I,J)
  SS(2,MM)=SS(2,MM)+P(1,N)*W(I,J)
  SS(4,MM)=SS(4,MM)+VD*W(I,J)
  SS(6,MM)=SS(6,MM)+0.5*(P(1,N)*P(1,N)+VD*VD+WD*WD)*W(I,J)
  SS(8,MM)=SS(8,MM)+1.
33  B=VMW*SQRT(-ALOG(RAN(I1,I2)))
  A=2.*PI* $RAN(I1,I2)$ 
  P2=B*SIN(A)
  P3=B*COS(A)
  P(1,N)=-VMW*SQRT(-ALOG(RAN(I1,I2)))
C THE MOLECULE IS REFLECTED WITH P(1,N),P(2,N) AND P(3,N)
  IF(MM.LE.0) GO TO 34
  SS(3,MM)=SS(3,MM)-P(1,N)*W(I,J)
  SS(5,MM)=SS(5,MM)+P2*W(I,J)
  SS(7,MM)=SS(7,MM)+0.5*(P(1,N)*P(1,N)+P2*P2+P3*P3)*W(I,J)
34  X=XM+P(1,N)*DTR
  R=SQRT((RD+P2*DTR)*(RD+P2*DTR)+P3*P3*DTR*DTR)
  P(2,N)=(P2*(RD+P2*DTR)+P3*P3*DTR)/R
  P(3,N)=P3*RD/R
  IF(R.GT.RM.OR.X.LT.0.) GO TO 54
35  CALL FINDCELL2(R1,X1,I,J)
  CALL FINDCELL2(R,X,K,L)
C (I,J) IS OLD CELL AND (K,L) IS NEW CELL
  P(4,N)=X
  P(5,N)=R
  IF(I.EQ.K.AND.J.EQ.L) GO TO 24
  B=W(I,J)/W(K,L)
  M=0
50  IF(B.LT.1.) GO TO 51
  M=M+1
  B=B-1.
  GO TO 50
51  A=RAN(I1,I2)
  IF(A.LT.B) M=M+1
  IF(M.EQ.0) GO TO 54
  IF(M.EQ.1) GO TO 24
C MOLECULE WILL BE DUPLICATED
  M=M-1
  DO 53 I=1,M
  NM=NM+1
  DO 52 J=1,5
52  P(J,NM)=P(J,N)
53  IP(NM)=-1
  GO TO 24
C MOLECULE WILL BE REMOVED
54  DO 55 I=1,5
55  P(I,N)=P(I,NM)
  IP(N)=IP(NM)
  NM=NM-1
  N=N-1
  GO TO 24
C MOLECULAR INDEXING
60  DO 61 J=1,NCX
  DO 61 I=1,NCR

```

```

        IC(1,I,J)=0
61      IC(2,I,J)=0
        DO 62 N=1,NM
        CALL FINDCELL2(P(5,N),P(4,N),I,J)
62      IC(1,I,J)=IC(1,I,J)+1
        M=0
        DO 64 J=1,NCX
        DO 64 I=1,NCR
        IC(2,I,J)=M
        M=M+IC(1,I,J)
        IC(1,I,J)=0
64      CONTINUE
C IC(1,I,J) IS THE NUMBER OF MOLECULES IN CELL (I,J)
C (IC(2,I,J)+1) IS THE STARTING ADDRESS IN CELL (I,J)
C MOLECULES WILL BE COUNTED IN R-DIRECTION FIRST, THEN IN X-DIR.
        DO 65 N=1,NM
        CALL FINDCELL2(P(5,N),P(4,N),I,J)
        IC(1,I,J)=IC(1,I,J)+1
        K=IC(2,I,J)+IC(1,I,J)
        LCR(K)=N
65      IP(N)=1
C CALCULATE COLLISIONS
        DO 79 J=1,NCX
        DO 79 I=1,NCR
        VRDT=C(2,I,J)
        NP=0
        MAX=IC(1,I,J)*(IC(1,I,J)+1)*100
        IF(C(1,I,J).GT.TIME) GO TO 79
        IF(IC(1,I,J).GE.2) GO TO 71
        C(1,I,J)=C(1,I,J)+DTM
        GO TO 79
C CHOOSE ONE MOLECULE OF COLLISION PAIR
71      NP=NP+1
        K=IC(2,I,J)+RAN(I1,I2)*IC(1,I,J)+0.9999999
        IF(K.EQ.IC(2,I,J)) K=K+1
        L=LCR(K)
C CHOOSE ANOTHER MOLECULE OF COLLISION PAIR
72      K=IC(2,I,J)+RAN(I1,I2)*IC(1,I,J)+0.9999999
        IF(K.EQ.IC(2,I,J)) K=K+1
        M=LCR(K)
        IF(L.EQ.M) GO TO 72
C CALCULATE RELATIVE VELOCITY COMPONENTS AND RELATIVE SPEED
        DO 73 K=1,3
73      VRC(K)=P(K,L)-P(K,M)
        VR=SQRT(VRC(1)*VRC(1)+VRC(2)*VRC(2)+VRC(3)*VRC(3))
        IF(VR.GT.VRDT) VRDT=VR
        A=VR/VRDT
        B=RAN(I1,I2)
        IF(NP.LE.MAX) GO TO 76
        C(1,I,J)=C(1,I,J)+DTM
        GO TO 79
76      IF(A.LT.B) GO TO 71
C COLLISION PROBABILITY IS PROPORTIONAL TO VR FOR HARDSPHERE MOLECULE
C ADVANCE CELL TIME AND COLLISION COUNTER
        C(1,I,J)=C(1,I,J)+2.*VL(I,J)/(IC(1,I,J)*IC(1,I,J)
        1 *CX*VR*W(I,J))
        MM=NN-NNN
        IF(MM.LE.0) GO TO 74
        SC(7,I,J,MM)=SC(7,I,J,MM)+1.
C CALCULATE POST COLLISION RELATIVE VELOCITY COMPONENTS
74      B=1.-2.*RAN(I1,I2)
        VRC(1)=B*VR
        A=SQRT(1.-B*B)
        B=2.*PI*RAN(I1,I2)
        VRC(2)=A*COS(B)*VR
        VRC(3)=A*STN(B)*VR

```

```

      DO 75 K=1,3
      VCCM=0.5*(P(K,L)+P(K,M))
C VCCM IS THE VELOCITY OF CENTER OF MASS
      P(K,L)=VCCM+0.5*VRC(K)
75      P(K,M)=VCCM-0.5*VRC(K)
C POST COLLISION VELOCITY COMPONENTS HAVE BEEN SET
      IF(C(1,I,J),LT,TIME) GO TO 71
79      CONTINUE
80      CONTINUE
C FLOW FIELD WILL NOW BE SAMPLED
      IF(MM.LE,0) GO TO 601
      DO 82 J=1,NCX
      DO 82 I=1,NCR
      K=IC(1,I,J)
      DO 82 N=1,K
      LL=IC(2,I,J)+N
      L=LCR(LL)
      SC(1,I,J,MM)=SC(1,I,J,MM)+1.
      SC(2,I,J,MM)=SC(2,I,J,MM)+P(1,L)
      SC(3,I,J,MM)=SC(3,I,J,MM)+P(2,L)
      DO 82 M=1,3
      SC(M+3,I,J,MM)=SC(M+3,I,J,MM)+P(M,L)*P(M,L)
82      CONTINUE
601     WRITE(6,600) NN,JJ
600     FORMAT(' NN=',I4,' JJ=',I4)
83     CONTINUE
      WRITE(6,84) NN
84     FORMAT(' END OF NN=',I3)
81     CONTINUE
C END OF SAMPLE ACCUMULATION
C FLOW PROPERTIES WILL NOW BE AVERAGED
      NNN=NSAM-NON
      AA=NST*NIS*DTM
      DO 89 NN=1,NNN
      OP(1)=SS(8,NN)
      OP(2)=SS(1,NN)
      A=AA*FND
      DO 88 I=3,9
88     OP(I)=SS(I-2,NN)/A
89     WRITE(4,90) NN,OP
90     FORMAT(1H ,I4,2F9.0,7F12.5)
      BB=AA*FND*CXS*SQRT(2./PI)
      DO 97 NN=1,NNN
      A=(NON+NN-1)*AA
      B=(NON+NN)*AA
      WRITE(4,91) A,B
91     FORMAT(' OFLOW FIELD PROPERTIES OVER THE TIME PERIOD FROM',
1 F12.5,' TO',F12.5/)
      WRITE(4,92)
92     FORMAT(' CELL SAMPLE DENSITY X-VEL. ',
1 ' Y-VEL. X-TEMP. Y-TEMP. Z-TEMP. ',
1 ' TEMP. COLL. RATE')
      WRITE(4,93)
93     FORMAT(' IR JX'/)
      DO 96 J=1,NCX
      DO 96 I=1,NCR
      OP(1)=SC(1,I,J,NN)
      OP(2)=SC(1,I,J,NN)/(NST*MC(I,J))
      OP(3)=SC(2,I,J,NN)/OP(1)
      OP(4)=SC(3,I,J,NN)/OP(1)
      OP(5)=2.*(SC(4,I,J,NN)/OP(1)-OP(3)*OP(3))
      OP(6)=2.*(SC(5,I,J,NN)/OP(1)-OP(4)*OP(4))
      OP(7)=2.*SC(6,I,J,NN)/OP(1)
      OP(8)=(OP(5)+OP(6)+OP(7))/3.
      OP(9)=SC(7,I,J,NN)/(BB*MC(I,J))
      WRITE(4,95) I,J,(OP(L),L=1,9)

```

```
95     FORMAT(1H ,2I4,F10.2,8F11.5)
96     CONTINUE
97     CONTINUE
      TIME=NSAM*NST*NIS*DTM
      WRITE(2,200) NM
200    FORMAT(I6)
      DO 201 J=1,NCX
      DO 201 I=1,NCR
201    C(1,I,J)=C(1,I,J)-TIME
      WRITE(2,202) ((C(1,I,J),I=1,NCR),J=1,NCX)
202    FORMAT(10E13.6)
      WRITE(2,203) ((C(2,I,J),I=1,NCR),J=1,NCX)
203    FORMAT(10E13.6)
      DO 205 J=1,NCX
      DO 205 I=1,NCR
      K=IC(1,I,J)
      DO 205 N=1,K
      LL=IC(2,I,J)+N
      L=LCR(LL)
      WRITE(2,204) (P(M,L),M=1,5)
204    FORMAT(5E13.6)
205    CONTINUE
      WRITE(2,206) ((IC(1,I,J),I=1,NCR),J=1,NCX)
206    FORMAT(10I5)
      STOP
      END
```

```
          SUBROUTINE FINDCELL2(R,X,I,J)
C  FOUR BLOCKS: #1(6*3), #2(4*3), #3(6*6), #4(4*6)
C  RM=7.0, XM=6.0, NCR=10, NCX=9
          PP=.9999999
          IF(X.GT.3.) GO TO 3
          IF(R.GT.3.) GO TO 2
          I=2.*R+PP
          J=X+PP
          GO TO 5
2          I=R+PP+3.
          J=X+PP
          GO TO 5
3          IF(R.GT.3.) GO TO 4
          I=2.*R+PP
          J=2.*X+PP-3.
          GO TO 5
4          I=R+PP+3.
          J=2.*X+PP-3.
5          IF(I.EQ.0) I=1
          IF(J.EQ.0) J=1
          RETURN
          END
```